

**PRAIRIE VIEW A&M UNIVERSITY
ROY G. PERRY COLLEGE OF ENGINEERING
DEPARTMENT OF CHEMICAL ENGINEERING
CHEG 4248-SENIOR DESIGN & PROFESSIONALISM II
SPRING 2022**

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Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

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Summary of Topics covered by Quiz

Original Quiz Questions & Master Solution/grading scheme used

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

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Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

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Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

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Summary of Topics Covered by Project

Project Problem Statement and Grading Scheme

Above Average (Graded original work)

Average (Graded original work)

Below Average (Graded original work)

[Include any other evaluation used and omit any method above method (Test, Quizzes, Homework, Laboratory and Project reports) that was not used]

(Note: All Pages shown in Yellow should be printed on YELLOW PAPER)

(Note: All Pages shown in Blue should be printed on BLUE PAPER)

Course Description in ABET Format

CHEG 4248: SENIOR DESIGN AND PROFESSIONALISM II

- | | |
|---|---|
| 1. Course number and name: | CHEG 4248: Senior Design and Professionalism II |
| 2. Credits, contact hours, categorization: | 2-Credit Hour, 4-Contact Hours, Engineering Topic |
| 3. Instructor's or course coordinator's name: | Dr. Emmanuel Dada |
| 4. Textbook: Title: | Not Required |
-
- | | |
|--------------------------------|---|
| Author: | |
| Publisher, Year & Edition: | |
| a. Other Supplemental material | <ol style="list-style-type: none">1. "Chemical Process Engineering: Design & Economics," by Harry Silla, 2003, Marcel Dekker, ISBN 0-8247-4274-5.2. "Analysis, synthesis and Design of Chemical Processes" by Richard Turton, Richard C. Bailie, Wallace B. Whitting, Joseph A. Schaeiwitz and Debangsu Bhattacharrya, 4th Edition, 2012, Prentice Hall, ISBN-13: 97801326181203. "Plant Design and Economics for Chemical Engineers" by Peters, M.S., K.D. Timmerhaus and R.E. West, 5th edition, 2003, McGraw-Hill, ISBN 0-07-2392665.4. "Fundamentals of Engineering Design", by Barry Hyman, 2nd edition, 2003, Pearson Education, Inc. (Prentice Hall), ISBN 0-13-046712-X5. "Chemical Engineering Process Design and Economics: A Practical Guide" by Gael D. Ulrich and Palligarnai T. Vasudevan, 2nd Edition, 2004, Process (Ulrich) Publishing, ISBN0-9708768-2-36. "Senior Project Manual" by Prairie View A & M University College of Engineering |
-
- | | |
|--|---|
| 5. Specific course information | |
| a. Brief description of the content of the course (catalog description) | CHEG 4248 (2:0) Credit 2 semester hours. This is the second course of a two-semester capstone experience (CHEG 4248 must immediately follow CHEG 4247 or the sequence must restart with CHEG 4247) involving the engineering design of an industrial or advanced team project. Elements of ethics and professionalism in engineering practice are integrated into the project experience. The project will include the application of relevant engineering codes and standards, as well as realistic constraints. Design achievements are demonstrated with written reports, oral presentations, professional standards, and ethics examinations. |
| b. Prerequisites | CHEG 3301, CHEG 3302, CHEG 3305, CHEG 3306, and CHEG 4247. |
| c. *Indicate whether a required, elective, or selected elective (as per definition provided) course in the program | Required |
| 6. Specific goals for the course | Students will be able to : |
| a. specific outcomes of instruction | <ol style="list-style-type: none">1. Be able to design a system, component, or process to meet desired needs.2. Demonstrate an understanding of professional and ethical responsibility.3. Be able to demonstrate the broad education necessary to understand the impact of engineering solutions in a global and societal context.4. Be able to recognize the need for and ability to engage in life-long |

learning.

5. Demonstrate knowledge of contemporary issues.

- b. Explicitly indicate which of the student outcomes listed in Criterion 3 or any other outcomes are addressed by the course.

This course addresses the following student learning outcome determined by the department:

Outcome 2:

Ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.

Outcome 3:

An ability to communicate effectively with a range of audiences.

Outcome 5:

Ability to (i) function effectively on a team whose memberstogether (ii) provide leadership, create a collaborative and inclusive environment, (iii) establish goals, plan tasks, and meet objectives.

7 Brief list of topics to be covered

1. Course overview & Manual: Meeting Agreement; Review of group dynamics.
2. Project constraints, tasks and GANTT charts.
3. Finalized Material/Energy balances and updated literature review.
4. Process design: Process simulation using HYSYS/ASPEN and Safety Review; Hazards, operability, and inherent safety (HAZOP analysis).
5. Design of major equipment, codes, and standards and HAZOP analysis.
6. Design equations and heuristics, codes, and standards.
7. Process Design and Analysis: Materials selection, equipment specification, and economic evaluation.
8. Capital costs, operating costs, and return on investment.
9. Final project presentation and report

Additional Course Syllabus Information

Information Item	Information
Instructor:	Dr. Emmanuel Dada
Section # and CRN:	P02 CRN 20557; P82 CRN 20558
Office Location:	C.L. Wilson 201 B
Office Phone:	936-261-9968
Email Address:	eadada@pvamu.edu ; emmanuel.dada@ymail.com
Office Hours:	Virtual: MWF 10:00 a.m. – 2:00 p.m.
Mode of Instruction:	Hybrid/Internet-(a)Synchronous Instructional Method
Course Location:	New Electrical Engr Bldg 115 (T); C L Wilson Engineering Bldg 109K (R)
Class Days & Times:	T 3:30 – 4:20 p.m.; R 3:30 - 6:20 p.m.

General Course Information Table

Access to Learning PVAMU

Resources:	Library:
phone: (936)	1500; web:
261- University	<u>http://www.tamu.edu/pvamu/library/</u>
	(936) 261-1990;
	web:
Bookstore:	<u>https://www.bkstr.com/Home/10001-10734-1?demoKey=d</u>
phone:	

Course Goals or Overview:

The goal of this course is to provide a capstone design experience for chemical engineering students who have completed all of their design coursework at the junior level and below.

Course Outcomes/Objectives

At the end of this course, the student will have achieved and demonstrated the following outcomes.

- 1 Be able to design a system, component, or process to meet desired needs.
- 2 Demonstrate an understanding of professional and ethical responsibility.
- 3 Be able to demonstrate the broad education necessary to understand the impact of engineering solutions in a global and societal context.
- 4 Be able to recognize the need for and ability to engage in life-long learning.
- 5 Demonstrate a knowledge of contemporary issues

Course Requirements & Evaluation Methods

This course will utilize the following instruments to determine student grades and proficiency of the learning outcomes for the course. Continuous assessment of students' homework assignments, oral presentations and written design reports will be used to evaluate their competence in ABET student outcomes 2 (ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors), 3 (an ability to communicate effectively with a range of audiences), and 5 (ability to

(i) function effectively on a team whose members together (ii) provide leadership, create a collaborative and inclusive environment, (iii) establish goals, plan tasks, and meet objectives).

Presentation – oral presentations, some of which are graded, to develop and demonstrate an ability to communicate effectively in oral mode.

Homework Exercises – **written assignments, often in letter report format, designed to supplement and reinforce course material. The letter report format serves to develop and demonstrate an ability to communicate effectively in written mode.**

Quizzes – **announced or surprise in-class assignments to promote student accountability** Project Report – **the central feature of this course is an open ended design project on a relevant, contemporary, technical problem in the student’s discipline. The report is the medium by which design accomplishments are demonstrated and also serves to develop and demonstrate an ability to communicate effectively in written mode.**

Class Participation – daily attendance and participation in class discussions

Grading Matrix (*points will vary according to instructor’s grading system*)

Instrument	Total
Homework Assignments	5%
Midterm progress report	5%
Final presentation	70%
Final project report	20%
Total	100%
Discount for lack of participation	-10%
<i>Extra credit (as assigned by instructor)</i>	

Grade Determination:

A = 100 –

90pts;

B = 89 – 80pts;

C = 70 –

79pts;

D = 60 –

69pts;

F = 59pts or below

Course Procedures

Textbook Policy

Students must acquire the textbook that is listed as “required” on the course syllabus. The textbook must be acquired by the 10th class day. Students are not allowed to share textbooks with other students who are currently registered in the same class. Failure to acquire (or show proof of purchase) the required textbook by the 10th class day will result in the student being administratively dropped from the course. The University will assess financial obligations for the course to the student as with any other dropped class according to the fee schedule. In addition, your financial aid may be affected by the subsequent registration action(s).

Go to <http://www.pvamu.edu/pages/195.asp> for the Roy G. Perry College of Engineering Textbook Policy.

Conduct:

1. Students will conduct themselves in a manner that is respectful to their fellow classmates and the instructor at all times.
2. **Cell phones, ipads and smart phones or similar electronic devices MUST** be turned off and stowed away during class time. Students are **NOT** allowed to leave class to answer cell phones or use these devices.
3. Students caught using ipads and smart phones or similar electronic devices during exams will receive **ZERO for the exam and be subject to sanctions as stipulated under Academic Misconduct.**
4. Students should be prepared to stay in the classroom for the duration of the exam. Students who have any condition that may require them to leave the exam room should make prior arrangements with the Instructor. Students who decide to leave the exam room for any other reason must hand over their exam paper and consider the exam over for them.
5. Programmable calculators are **NOT** allowed in class.

6. Students should dress professionally and are **NOT** allowed to wear caps/hats in class.
7. Students are NOT allowed to bring food to the classroom or eat in class
8. Arrive to class prepared to discuss lesson with your project binder.

Submission of Assignments:

There will be project assignments, reports and presentations. All presentations will be team presentations and each student is required to contribute to the success of the team. It is recommended that a member of the group be assigned the duty of recorder, and maintain the minutes of meetings (with listing of attendees) and a notebook with pertinent information. Individual reports are to be submitted at mid term and at the end of the semester detailing the contribution of each team member. A team report is to be submitted at midterm and a final report

is to be submitted **at the end of the semester.** In the event that it becomes necessary to remove a member from a team, the following procedure must be followed:

- The team minus the affected member, must meet to discuss the action to be taken.
- The team must then meet with the affected student and discuss the action to be taken.
- A letter must be submitted to the instructor giving justification for the action to be taken. The letter must be signed by all team members and a copy must be sent to the affected student.
- The instructor will then schedule a meeting with the team members and the affected student for final discussion and appropriate action.

*All homework assignments are due directly to the Instructor, prior to the start of class or the assignment will not be accepted. All homework assignments and exams should be written on one side of the page only, and should use the appropriate cover sheet, with the name, assignment title and date. All pages should be numbered. Failure to use the correct cover sheet will result in the assignment grade being reduced by 20%. **Formatting Documents:** Microsoft Word is the standard word processing tool used at PVAMU. If you're using other word processors, be sure to use the "save as" tool and save the document in either the Microsoft Word, Rich-Text, or plain text format. **Exam Policy***

Exams should be taken as scheduled. No makeup examinations will be allowed except under documented emergencies (See Student Handbook).

Professional Organizations and Journals

As directed by instructor.

References

As directed by instructor.

16 WEEK CALENDAR

Week One: Topic	Course overview & Manual: Meeting Agreement; Review of group dynamics
Chapter (s):	
Assignment (s):	Reading: Group dynamics
Week Two: Topic	Project constraints, tasks and GANTT chart
Chapter (s):	
Assignment (s):	Homework 1: Group dynamics and GANTT chart
Week Three: Topic	Finalized Material/Energy balances and updated literature review
Chapter (s):	
Assignment (s):	Homework 2
Week Four: Topic	Process design: Process simulation using HYSYS/ASPEN and Safety Review; Hazards, operability and inherent safety (HAZOP analysis)

Chapter (s):
Assignment (s): Homework 3

Week Five: Topic Design of major equipment, codes and standards and HAZOP analysis
Chapter (s):
Assignment (s): Reading: Design equations and heuristics, codes and standards

Week Six: Topic Design of major equipment, HAZOP analysis
Chapter (s):
Assignment (s): Homework 4

Week Seven: Topic Design of major equipment
Chapter (s):

Assignment (s): Reading: Codes and standards

Week Eight: Topic Design of major equipment
Chapter (s):
Assignment (s): **Mid Term**

Week Nine: Topic
Chapter (s):
Assignment (s): **Spring Break**

Week Ten: **Topic Process Design and analysis: Materials selection**
Chapter (s):
Assignment (s): Reading: Materials selection

Week Eleven: **Topic Process Design and analysis: Equipment specification**
Chapter (s):
Assignment (s): Reading: Mechanical engineering design and Plant layout

Week Twelve: **Topic Process Design and analysis: Process control; final safety review and HAZOP analysis**
Chapter (s):
Assignment (s): Reading: Process control and instrumentation

Week Thirteen: **Topic Process Design and analysis: Economic Evaluation**
Chapter (s):
Assignment (s): Capital costs, operating costs and return on investment

Week Fourteen: **Topic Process Design and Analysis: Outline of project presentation**
Chapter (s):
Assignment (s): Completion of detailed plant design

Week Fifteen: Topic Course
Review
Chapter (s):
Assignment (s): Final draft of project report due

Week Sixteen **Final Presentation; Final Report due**

University Rules and Procedures

Disability statement (See Student Handbook):

Students with disabilities, including learning disabilities, who wish to request accommodations in class should register with the Services for Students with Disabilities (SSD) early in the semester so that appropriate arrangements may be made. In accordance with federal laws, a student requesting special accommodations must provide documentation of their disability to the SSD coordinator.

Academic misconduct (See Student Handbook):

You are expected to practice academic honesty in every aspect of this course and all other courses. Make sure you are familiar with your Student Handbook, especially the section on academic misconduct. Students who engage in academic misconduct are subject to university disciplinary procedures.

Forms of academic dishonesty:

1. Cheating: deception in which a student misrepresents that he/she has mastered information on an academic exercise that he/she has not mastered; giving or receiving aid unauthorized by the instructor on assignments or examinations.
2. Academic misconduct: tampering with grades or taking part in obtaining or distributing any part of a scheduled test.
3. Fabrication: use of invented information or falsified research.
4. Plagiarism: unacknowledged quotation and/or paraphrase of someone else's words, ideas, or data as one's own in work submitted for credit. Failure to identify information or essays from the Internet and submitting them as one's own work also constitutes plagiarism.

Nonacademic misconduct (See Student Handbook)

The university respects the rights of instructors to teach and students to learn. Maintenance of these rights requires campus conditions that do not impede their exercise. Campus behavior that interferes with either (1) the instructor's ability to conduct the class, (2) the inability of other students to profit from the instructional program, or (3) campus behavior that interferes with the rights of others will not be tolerated. An individual engaging in such disruptive behavior may be subject to disciplinary action. Such incidents will be adjudicated by the Dean of Students under nonacademic procedures.

Sexual misconduct (See Student Handbook):

Sexual harassment of students and employers at Prairie View A&M University is unacceptable and will not be tolerated. Any member of the university community violating this policy will be subject to disciplinary action.

Attendance Policy:

Prairie View A&M University requires regular class attendance. Excessive absences will result in lowered grades. Excessive absenteeism, whether excused or unexcused, may result in a student's course grade being reduced or in assignment of a grade of "F". Absences are accumulated beginning with the first day of class.

Student Academic Appeals Process

Authority and responsibility for assigning grades to students rests with the faculty. However, in those instances where students believe that miscommunication, errors, or unfairness of any kind may have adversely affected the instructor's assessment of their academic performance, the student has a right to appeal by the procedure listed in the Undergraduate Catalog and by doing so within thirty days of receiving the grade or experiencing any other problematic academic event that prompted the complaint.

Technical Considerations for Online and Web-Assist Courses

Minimum Hardware and Software Requirements:

- Pentium with Windows XP or PowerMac with OS 9

- 56K modem or network access

- Internet provider with SLIP or PPP

- 8X or greater CD-ROM

- 64MB RAM

- Hard drive with 40MB available space

- 15" monitor, 800x600, color or 16 bit

- Sound card w/speakers
- Microphone and recording software
- Keyboard & mouse
- Netscape Communicator ver. 4.61 or Microsoft Internet Explorer ver. 5.0 /plug-ins

Participants should have a basic proficiency of the following computer skills:

- Sending and receiving email
- A working knowledge of the Internet
- Proficiency in Microsoft Word
- Proficiency in the Acrobat PDF Reader
- Basic knowledge of Windows or Mac O.S.

Netiquette (online etiquette): students are expected to participate in all discussions and virtual classroom chats when directed to do so. Students are to be respectful and courteous to others in the discussions. Foul or abusive language will not be tolerated. When referring to information from books, websites or articles, please use APA standards to reference sources.

Technical Support: Students should call the Prairie View A&M University Helpdesk at 936-261-2525 for technical issues with accessing your online course. The helpdesk is available 24 hours a day/7 days a week. For other technical questions regarding your online course, call the Office of Distance Learning at 936-261-3290 or 936-261-3282

Communication Expectations and Standards:

All emails or discussion postings will receive a response from the instructor within 48 hours.

You can send email anytime that is convenient to you, but I check my email messages continuously during the day throughout the work-week (Monday through Friday). I will respond to email messages during the work-week by the close of business (5:00 pm) on the day following my receipt of them. Emails that I receive on Friday will be responded to by the close of business on the following Monday.

Submission of Assignments:

Assignments, Papers, Exercises, and Projects will distributed and submitted through your online course. Directions for accessing your online course will be provided. Additional assistance can be obtained from the Office of Distance Learning.

Discussion Requirement:

Because this is an online course, there will be no required face to face meetings on campus. However, we will participate in conversations about the readings, lectures, materials, and other aspects of the course in a true seminar fashion. We will accomplish this by use of the discussion board.

Students are required to log-on to the course website often to participate in discussion. It is strongly advised that you check the discussion area daily to keep abreast of discussions. When a topic is posted, everyone is required to participate. The exact use of discussion will be determined by the instructor.

It is strongly suggested that students type their discussion postings in a word processing application and save it to their PC or a removable drive before posting to the discussion board. This is

important for two reasons: 1) If for some reason your discussion responses are lost in your online course, you will have another copy; 2) Grammatical errors can be greatly minimized by the use of the spell-and-grammar check functions in word processing applications. Once the post(s) have been typed and corrected in the word processing application, it should be copied and pasted to the discussion board.

Video Conferencing Etiquette

When using Zoom, WebEx or other video conferencing tools, confirm the visible area is tidy, clear of background clutter, inappropriate or offensive posters, and other distractions. Ensure you dress appropriately and avoid using high traffic or noisy areas. Stay muted when you are not speaking and avoid eating/drinking during session. Before class session begins, test audio, video and lighting to alleviate technology issues. Technical Support

Students should go to the [Password Reset Tool](#) if they have password issues. The page will provide instructions for resetting passwords and contact information if login issues persist. For other technical questions regarding eCourses, call the Center for Instructional Innovation and Technology Services (CIITS) at 936-261-3283 or email ciits@pvamu.edu.

Communication Expectations and Standards

Emails or discussion postings will receive a response from the instructor, usually in less than 48 hours. Urgent emails should be marked as such. Check regularly for responses.

Discussion Requirement

Online courses often require minimal to no face-to-face meetings. However, conversations about the readings, lectures, materials, and other aspects of the course can take place in a seminar fashion. This will be accomplished by the use of the discussion board. The exact use of discussion will be determined by the instructor.

It is strongly suggested that students type their discussion postings in a word processing application such as Word and save it to their PC or a removable drive before posting to the discussion board. This is important for two reasons: 1) If for some reason your discussion responses are lost in your online course, you will have another copy; 2) Grammatical errors can be greatly minimized by the use of the spell-and-grammar check functions in word processing applications. Once the post(s) have been typed and corrected in the word processing application, copy and paste to the discussion board.

COVID-19 Campus Safety Measures

To promote public safety and protect students, faculty, and staff during the COVID-19 pandemic, Prairie View A&M University has adopted policies and practices for the Fall 2020 academic term to limit virus transmission. Students must observe the following practices while participating in face-to-face courses and course-related activities (office hours, help sessions, transitioning to and between classes, study spaces, academic services, etc.):

- **Self-monitoring** - Students should follow CDC recommendations for self-monitoring. Students who have a fever or exhibit symptoms of COVID-19 should participate in class remotely and should not participate in face-to-face instruction.
- **Face Coverings** - Face coverings (cloth face covering, surgical mask, etc.) must be properly worn in all non-private spaces including classrooms, teaching laboratories, common spaces such as lobbies and hallways, public study spaces, libraries, academic resource and support offices, and outdoor spaces where 6 feet of physical distancing is difficult to reliably maintain.
- **Physical Distancing** - Physical distancing must be maintained between students, instructors, and others in course and course-related activities.
- **Classroom Ingress/Egress** - Students must follow marked pathways for entering and exiting classrooms and other teaching spaces. Students should leave classrooms promptly after course activities have concluded, should not congregate in hallways and should maintain 6-foot physical distancing when waiting to enter classrooms and other instructional spaces.
- **Face-to-face Class** - To attend a face-to-face class, students must wear a face covering (or a face shield if they have

an exemption letter). If a student refuses to wear a face covering, the instructor should ask the student to leave and join the class remotely. If the student does not leave the class, the faculty member should report that student to the Office for Student Conduct for adjudication. Additionally, the faculty member may choose to teach that day's class remotely for all students.

- **COVID-19 Guidelines for Student Conduct Adjudication** - The mandatory COVID-19 Training/Certification taken by all students serves as the 1st Warning for violation of COVID-19 Guidelines.
 - 1st incident: upon review of Incident Report and finding of responsibility — Conduct Probation
 - 2nd incident: upon review of Incident Report and finding of responsibility — Suspension
 - Consult the Code of Student Conduct in the Student Planner or [Student Conduct website](#) for additional information on Conduct Probation and Suspension.
- **Personal Illness and Quarantine** - Students required to quarantine must participate in courses and course-related activities remotely and must not attend face-to-face course activities. Students should notify their instructors of the quarantine requirement. Students under quarantine are expected to participate in courses and complete graded work unless they have symptoms that are too severe to participate in course activities. Students experiencing personal injury or illness that is too severe for the student to attend class qualify for an excused absence. To receive an excused absence, students must provide appropriate documentation to the Office for Student Conduct, studentconduct@pvamu.edu.

II ASSESSMENT RESULTS FOR CURRENT AND PAST THREE PERIODS

Program Outcomes Assessed in this course

Outcome 1:

An ability to identify, formulate, and solve complex engineering problems (CEP) by applying principles of engineering, science, and mathematics.

Outcome 6:

An ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions.

Assessment Summary of Class Semester Averages for Outcomes (Should be provided for Spring 2021 through Spring 2022 Assessment Period)

Outcomes	2	3	5
Semester	Semester Class Average (%)	Semester Class Average (%)	Semester Class Average (%)
Spring 2022	83	83	86
SPRING 2021	83	85	86
Comments on Trend of Data (Improving or deteriorating)	Students' performance over the two-semester period was above the expected average. And for both semesters, there is a slight improvement from 2021 avg 82.6% to 2022 semester avg 83%.	91 % of students in the 2022 spring semester met the expected class average better than 85% of students in spring semester that met the expected average.	Students' performance over the two-semester period was above the expected average. And for both semesters, there is a slight improvement from 2021 avg 85.6% to 2022 semester avg 86.4%.

*Expected Semester Class Average = 70% (or as defined by the program)
Ideal Semester Class Average = 75% (or as defined by the program)

End of Semester Course Assessment Reports Spring 2022 and Last Three Assessment Periods.

Each summary contains the following Information

1. Performance Statistics

- Total number of students in class
- The class average performance (**stated as %**) in each course outcome assessed in this class and the **two previous times course was assessed**.
- The acceptable class average for the class in each outcome area as set by your Department.
- Percentage of students who scored below the expected average in each outcome.

2. Implementation Summary

- Brief summary of plans implemented during the semester based on last assessment report

3. Perceived Problems

- Instructor's **critical evaluation** of perceived problems that affected students' performance. **Realistic problems should be identified throughout the semester and summarized in this section of the report.**

4. New Plans for Addressing Problems

- Instructor's plans for addressing the perceived problems the next time the class is taught. **These should be specific enough for another instructor to implement. Most of these should be things that, you, the instructor can implement to help students to improve. Be creative.**

5. Overall Trend over last three assessment periods

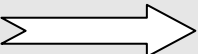
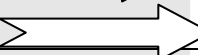
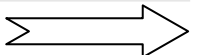
- Instructors summary of overall performance trend for each outcome measured over the last three periods.

5. Were Expectations Met?

- Answer **YES** if the **class average was above the expected average** and the **stated percentage of students** scored at or above the expected average, else answer NO.

END OF SEMESTER COURSE OUTCOME ASSESSMENT REPORT CHEG 4482-P02
SENIOR DESIGN & PROFESSIONALISM II SPRING 2022 SEMESTER

Report Prepared by: Dr. Emmanuel A. Dada Date: July 14, 2022

Semester	Analysis Type	Number of Students	Outcome 2 Ability to design a system, component or process				Outcome 3 Oral and written communication skills				Outcome 5 Ability to function in multi-disciplinary teams			
			Expected Class Average	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average	Expected Class Average	Expected Percent of students at or above average	Class Average	% Students meeting Expected Average
Spring 2022	Direct	22	75	70	83	100	75	70	83	91	75	70	86	100
Spring 2021	Direct	26	75	70	83	100	75	70	85	85	75	70	86	100
Implementation Summary			Items implemented from previous report or after meeting previous instructor 				-Lectures given to cover the design of major equipment -Review codes for pressure vessel and heat exchanger design -Classes coordinated with the PVAMU Library in Fall 2019 to teach student how to locate and use reference materials				Students were required to submit progress report drafts throughout the semester along with a rough draft of the final report. Corrections and feedback were provided to the students in time for them to make edits before the final submission.			
Perceived Problems			Perceived problems are directly related to the PC and the sub items under them 				-Students have difficulty applying relevant design equations to process components in the proper units -Students have a weak sense of correct order magnitude for correct sizing				Some grammatical errors and some students not following instructions on how to write summaries and the use of the College of Engineering Senior Design Report Manual partly affected report quality.			
Plans for Addressing Problems			Plans for address specific measures to address PC and their sub areas 				Recommendations: -Continue to assign component design homework problem in the early part of the semester -Add a design assignment at the end of CHEG 4472 (Fall semester) on a simpler system (HEX or pressure changer) for students to gain experience				The instructor should: Continue to require draft reports and progress reports to students to critique and identify strong and weak points and how grammar, clarity and organization could be improved.			
			Recommendations: -Continue to require student confidential group evaluations. -Utilize individual assessments where there is an opportunity -Continue to have team leaders submit weekly records of meeting minutes and summaries of completed tasks and action items.											

Overall Trend over Periods	Ascertain if there were improvements over previous semesters	Students' performance over the two-semester period was above the expected average. And for both semesters, there is a slight improvement from 2021 avg 82.6% to 2022 semester avg 83%.	91 % of students in the 2022 spring semester met the expected class average better than 85% of students in spring semester that met the expected average.	Students' performance over the two-semester period was above the expected average. And for both semesters, there is a slight improvement from 2021 avg 85.6% to 2022 semester avg 86.4%.
Were Expectations Met?	Class Average $\geq 75\%$ and $\geq 70\%$ of Students Performed at or Above Expected Average.	YES	YES	YES

**CHEMICAL ENGINEERING SENIOR DESIGN &
PROFESSIONALISM II
SPRING 2022**

Title of Assignment: Final Project Report

SENIOR DESIGN AND PROFESSIONALISM II

SPRING 2022

End of Semester Project Report Format

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1. Letter of Transmittal

The letter of transmittal captures the main points in in the EXECUTIVE SUMMARY.

(i) It clearly spells out why the report has been prepared.

(ii) Essential results, conclusions and recommendations are presented

See your College of Engineering Senior Design Manual for an example.

2. The EXECUTIVE SUMMARY

Your Executive Summary is a carefully distilled form of your complete design report and should have the following components:.

(a) It should clearly state the need for the design and its objectives

(b) It should clearly summarize what was done and main findings (process and production capacity, plant location and plant design and capital cost estimates, the capital investment , return on investment including, discounted cash flow internal rate of return, payback period etc)

(c) How the final results were obtained

(d) Clearly presented conclusions and recommendations.

Design Constraints and Design Basis

External constraints:

1. Physical laws

2. Standards and codes

3. Economic

4. Government and safety regulations
5. Resources

Internal constraints:

1. Choice of process
2. Process conditions
3. Materials and equipment
4. Time (for completion of design)
5. Personnel

Setting the Design Basis

1. Production rate
2. Purity specifications of the main product
3. The system of units to be used
4. The national, local, or company design codes that must be followed
5. Details of raw materials that are available
6. Information on potential sites where the plant might be located, including climate data, seismic conditions, and infrastructure availability
7. Information on the conditions, availability, and price of utility services such as fuel gas, steam, cooling water, process air, process water, and electricity that will be needed to run the process

The grading rubrics for evaluation of the Senior Design II projects CHEG 4248 (a continuation of the the fall 2021 Senior Design I CHEG 4247) are presented below. The students are to be evaluated as outlined in the rubrics with emphasis on the following:

-
- Justification of plant location and capacity
 - Provide a process description and Process Flow Diagram (PFD) for the plant showing the major items of equipment, and indicating the materials of construction and the operating temperatures and pressures
 - Material and energy balances with summary table for the process with streams information showing a mass balance for each major equipmentt
 - A complete HYSYS/ASPEN simulation report of the process
 - Chemical engineering design of major equipment such as (i) reactor(s), (ii) absorption column(s) and (iii) dsistillation columns
 - Estimates of the Major Equipment Capital Cost (Capex)
 - Estimates of Operating Cost (Opex)
 - Preparation of a net present value and investor's rate of return analysis for the investment over a 15-year life, assuming the company's current capital hurdle rate is 15%.
 - Preparation of a project milestone schedule
 - Preparation of a P&ID for a section of the process showing the control scheme to ensure safe operation of the unit, and carrying out a HAZOP analysis of the section of the process selected
 - Preparation of a safety report indicating the safety measures required for the plant bearing in mind any toxic and flammable materials handled
-

In addition, the names of the presenters for each design project have been included in the rubrics to enable each presenter to be evaluated as well.

References:

- 1. Gael D. Ulrich and Palligarnai T. Vasudevan, “ Chemical Engineering : Process Design and Economics, A pratical Guide”, second edition, 2004, Process Publishing, New Hampshire,USA, ISBN 0-9708768-2-3**
 - 2. Gavin Towler and Ray innott, “Chemical Engineering Design : Principles, Practice and Economics of Plant and Process Design” Butterworth-Heinemam, ISBN 978-0-08-096659-5, second edition, 2013**
 - 3. Perry’s Chemical Engineering Handbook, sith edition or latest**
-
- 4. Turton, R., Bailie, R., Whiting, W., and Shaeiwits, J. A. “Analysis, Synthesis, and Design of Chemical Processes,” 4th Edition Prentice-Hall PTR, Upper Saddle River, New Jersey 07458, 2008.**
 - 5. “Plant Design and Economics for Chemical Engineers” by Peters, M.S., K.D. Timmerhaus and R.E. West, 5th edition, 2003, McGraw-Hill, ISBN 0—07-239266-5.**

DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM II CHEG 4248
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR SPRING 2022 SEMESTER

ABET Student Learning Outcome 2: An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factor.
Assignments that test competency in this area will include problems testing students' understanding of the design process involving *devising a system, component, or process to meet desired needs and specifications within constraints, through an iterative, creative, decision-making process in which the basic sciences, mathematics, and engineering sciences are applied to convert resources into solutions.*

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Points Assigned	Points Received
1. Ability to Define/Understand the Problem and then Plan the Project	60	
(i) Identify the customer and the needs.	8	
(ii) Identify and list the design objectives.	8	
(i) Identify the design constraints.	4	
(ii) Define the design strategy and methodology.	4	
(iii) Identify and break down work into tasks and subtasks and identify the personnel and deliverables for each.	20	
(iv) Develop a Gantt chart and critical path analysis for managing the project.	8	
(v) Establish major milestones for tracking progress and define performance metrics to measure success	8	
2. Ability to Conduct a Review of the Literature	80	
(i) Identify the types of information needed for a complete understanding of all aspects of the project (Based on task described in the project planning).	20	
(ii) Gather information on relevant fundamentals, theory / concept (demonstrate technical competence) and relate them to the design.	40	
(iii) Provide the sources in a list of references properly cited in the literature review section and relevant sections of the report.	20	
3. Ability to perform preliminary design by generation of ideas and applying creativity through generation of ideas and evaluation of candidate solutions	60	
(i) Perform process design and analysis with design constraints; Sorting/screening of process technology alternatives based on availability and cost of raw materials, reaction selectivity and yield, thermodynamic barriers to separating undesired components, and safety and operability	40	
(ii) Evaluate candidate solutions to arrive at feasible designs	20	
4. Ability to Perform Preliminary and Detailed Design	200	
(i) Prepare a process flow diagram (PFD) and present a detailed description of the process indicating the functions of the major equipment components and controls, stream connectivity, safety, and other technical matters of importance	20	
(ii) Carry out a HYSYS/ASPEN simulation of the process showing a converged HYSYS/ASPEN model of the process. State assumptions/parameters used in modeling major equipment	20	
(ii) Prepare a chemical engineering design of (i) reactor(s), (ii) absorption column(s) and (ii) product distillation units, stating the materials of construction and the operating temperatures and pressures	60	
(iii) Prepare mechanical engineering design of the reactor(s) and distillation columns with appropriate dimensioned sketches	20	
(iii) Identify applicable codes and standards for the chemical and mechanical engineering designs. Indicate assumptions made and their justification, and support calculations should be in consistent units; either English Units or SI. Indicate possible sources of error	20	
(iv) Economic Evaluation: Estimate capital costs including engineering, materials, installation, interest, return on investment, taxes and contingency. Total unit conversion cost of product, a sensitivity study on the price of the raw material, and the economic methods used should be included	30	
(v) Prepare a control scheme to ensure safe operation of the plant and carry out Safety Reviews; Hazards, operability and inherent safe (including the use of Safety Data Sheets submitted in the Appendix) or HAZOP analysis	30	
Total	400	

ABOVE AVERAGE

(Note: All Pages shown in Light Blue should be printed on Light Blue Paper)

**Above Average Student Original Graded Assignment on Final Project
Report**

THE PRODUCTION OF DIMETHYL ETHER

87%

Taylon Owens

Amiya Rogers

Cinthia Sahin

Laura Ukpede

Senior Design Report

Spring 2022

Department of Chemical Engineering

Prairie View A&M University

Faculty Advisor: Dr. Emanuel Dada, Prairie View A&M University

May 3, 2022

Letter of Transmittal

May 3, 2022

Department of Chemical Engineering
Prairie View A&M University
100 University Dr,
Prairie View, TX 77446

Dear Dr. Dada,

As it pertains to our senior design problem statement, we have successfully completed our analysis of the production of dimethyl ether (DME) comes through the dehydration of methanol. We conclude that this method is a more efficient way to produce dimethyl ether versus the other alternatives that were evaluated. The project has the goal of producing 50,000 metric tons per year from a plant that will be based in Plaquemine, Louisiana. This is achieved by sourcing methanol at a relatively subsidized price and using efficient processes to produce DME at a purity level of over 90%. The high quality of DME produced, and the incorporation of a recycling stream and wastewater treatment for other uses means that the process has been determined to not only be economically viable, but also environmentally sustainable.

The report presented here thus expounds on the processes that were undertaken to complete the project objectives in coherence with the realized problem statement. In this regard, the report defines the project's scope and then details how it was planned and the delegation of tasks. The report also contains a literature review section which expounds on previous work that has been done in the production of DME, and how this work presented relevant resources and reference points for the completion of the project. Other sections of the report include process selection and description, the relevant energy and material balances for the chosen process, a discussion of how the process was completed, and finally recommendations for the production of DME in the future.

Four team members were involved in carrying out various tasks to complete the project's objectives. These members are Taylon Owens, Amiya Rogers, Cinthia Sahin and Laura Ukpede. Throughout the course of the project, ~~the~~ team leader, Taylon Owens, assigned specific roles to team members and coordinated each member's efforts to ensure that deliverables were completed within the stipulated timeframe. The estimated overall profit were \$23MM with a 22% return on investment. Consequently, all the project's goals were realized within the given time of eleven (11) weeks. The processes undertaken to accomplish this are thus elaborated in the succeeding report.

OLC

Taylon Owens

Amiya Rogers

Cinthia Sahin

Laura Ukpede

Abstract

The Production of 50,000 metric ton dimethyl ether (DME) was designed by using the dehydration method of methanol. Methanol is fed into a recycle stream and is fed into a reactor where dehydration occurs and produces DME and water. Once this is done, the existing stream is fed into a distillation column that produces DME as product in the distillate and a mixture of methanol and water in the bottoms. The bottoms stream is fed to another distillation column where the remaining methanol is recycled back into the feed and the bottoms stream is disposed of as wastewater. Within this design process one main assumption is considered. The design process assumed to be at 90% conversion.

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1. Project Scope

1.1 Problem Statement

The purpose of this project is to design a system that produces dimethyl ether (DME) at the required 99.9% purity.

1.2 Client Identification and Recognition of Need

For our process we decided that it would be best to get our methanol from the gulf coast which will cost us \$359.00 per metric ton. The reasoning behind this, is because methanol purchased from the gulf coast is relatively cheaper and the gulf coast is transportation hub which would make transporting our product (DME) easier. Once we purchase the methanol, we plan to use to produce 50,000 metric ton of DME per year through the process of methanol dehydration. Once the DME is produced, we plan to sell to Ford, FPT, Powertrain, and China at \$900.00 per metric ton.

1.3 Project Goals and Objectives

For this project we decided it would be best to list out important tasks that would progress our process along. We first started with understanding our process which led us to figuring out parameters regarding major equipment there after we shifted our focus to our process design where we devolved our process flow diagram and overall material balance. Lastly we wrapped up our project by creating a cost analysis followed by safety consideration. Each of the following major tasks were split into phases and sub tasks.

1.4 Contemporary issues and impact of project on society

The production of dimethyl ether is a relatively eco-friendly process being that global warming potentials are low compared to chlorofluorocarbons which are traditionally coolants. However high exposure can lead to headaches, dizziness, light headedness, and even loss of consciousness. Also, it is highly flammable and can cause fires. With this being said, the process of Methanol Dehydration was the best option for our team.

2. Project Planning and Task Identification

2.1 Task Identification

The following is the list of tasks that was delegated to our process. HYSYS/ASPEN simulation of process, chemical engineering design, economic evaluation, safety and hazop analysis, overall report, visual & oral presentation.

2.2 Timelines

In order to ensure all tasks were accomplished, it was important to identify major tasks and subtasks. This allowed for maximum productivity and ensured project completion. The use of a Gantt chart provided a visual reference of what needed to be completed and by when. Table 1 and Figure 1 detail the organization of the project over the course of the semester.

Table 1: Overview of Project Completion

Task	Time period
HYSYS/ASPEN Simulation	Feb. 18-25
Chemical Engineering Design	Feb. 28-March.28
Economic Evaluation	March. 30-April 13
Safety and Hazop Analysis	March. 30-April 13
Finish report	April. 9-16

Above is the identification of the major tasks needed to complete the project and the dates by which each should be completed.

[illegible]

Above is the Gantt chart that details the major tasks and subtasks. As shown, the anticipated completion date and duration for each task is listed.

This section of the report gives an overview of the manufacturing processes pertinent to DME. The section also examines DME's production routes, its physical and chemical properties, as well as safety aspects including handling and storage.

3.1. Overview of Manufacture of DME

Dimethyl ether (DME) is an organic compound that is well-known as a propellant and coolant. It can be used as an alternative fuel for diesel engines, due to its relatively low carbon footprint and high-performance characteristics. In normal conditions, DME presents as a colorless gas and liquifies at about 75 psi ("Alternative Fuels Data Center: Dimethyl Ether", n.d.). Other applications of DME include; as a solvent, an aerosol and a refrigerant.

The production of DME encompasses various sources including; biomass, fossil fuels and methanol. In the U.S., the idealized source for the production of DME is natural gas. The most common means of production for DME encompasses synthesis from syngas generated from fossil fuels.

The molecular formula for DME is thus presented as CH_3OCH_3 , which can consequently be simplified to $\text{C}_2\text{H}_6\text{O}$.

3.2. Production Routes

There are two distinctive routes for the production of DME entailing, the indirect route and the direct route. The indirect route involves the dehydration of methanol which is readily available to produce DME. On the other hand, the direct route involves the production of syngas from a variety of sources, which can then be converted to methanol and then to DME. These production routes are examined in details in the following sections.

3.2.1. Indirect Synthesis Route

The indirect synthesis of DME takes a more traditional approach whereby, methanol is obtained from a variety of sources, purified and then converted to DME (Azizi et al., 2014). As

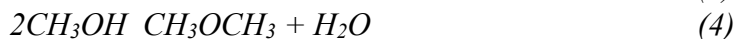
stated above, this production route fundamentally involves the dehydration of methanol resulting in the production of DME, and water as a by-product. This process is given by the following reaction.



According to Azizi et al., (2014), the most preferred method of methanol dehydration to produce DME involves a solid-acid catalyst and involves either the Langmuir-Hinshelwood or Eley-Rideal kinetic models. In both these models, water and DME act as reaction inhibitors at temperatures of above 300°C and therefore, this production route is favored at lower temperatures (Azizi et al., 2014).

3.2.2. Direct Synthesis Route

Recent research and technology have developed means of synthesizing DME directly from syngas using a single reactor. This process encompasses the formation of methanol, a water-gas shift, and methanol dehydration (Falco, 2021). This series of process is presented as follows includes; methanol formation, water-gas shift, methanol dehydration, and the overall reaction.



In the reactions above, both the formation of methanol and the water-gas shift occur within the overall process of converting syngas to DME. The formation of methanol is crucial in the synthesis of DME, whereas water-gas shift produces CO₂ which can then be recycled and use in reforming methane, and consequently syngas. The recycling of CO₂ with methane to produce syngas is given by the following reaction (Azize et al., 2014).



The direct synthesis of DME from syngas is a highly exothermic reaction and measures should be put in place to regulate temperature and prevent run-away. This production although being relatively more efficient, involves a complicated process and is thus more costly and resource intensive.

A summary of the process routes considered for this project is presented in the following table.

Table 2: Characteristics of Each Alternative

ALTERNATIVE	PROCESS	PROS	CONS
1	Methanol Dehydration	- Consumes less time and cost of equipment -Catalyst deactivation occurs at relatively high temp (400C). -Relatively simpler process flow	-Requires more downstream separation technologies -Sourcing of methanol may present challenges. -Marginally lower DME yield
2	Indirect Synthesis from biogas feedstock	-Marginally higher yield of DME -The risk of water build up in the process is alleviated -Energy Efficiency is maximized	-Sourcing of biogas feedstock presents a challenge. -Process requires more equipment. -Relatively Costly and time-consuming
3	Direct Synthesis from Natural Gas Feed Stock	-Higher yield of DME in comparison to methanol dehydration. -No risk of water build-up	-Exothermic reaction may lead to runaway reaction. -Catalyst deactivation at temp above 300C -Relatively more costs and time-consuming.

3.3. Physical and Chemical Properties

At atmospheric pressure and room temperature, DME presents as an odorless, colorless gas. Under severe or prolonged exposure to heat, any DME containers rupture violently ("Dimethyl ether", n.d.). DME has several other physical properties, some of which are summarized in the following table ("Fundamental Aspects of Dimethyl Ether", n.d.).

Table 3: DME Properties

Property	Value
Molecular weight	46.07
Boiling point	248.3 K
Freezing point	131.7 K
Critical pressure	52.5 atm
Critical Temperature	402.0 K
Heat of melting	25.6 cal/g
Heat of vaporization	111.6 cal/g
Specific Heat @ 248 K	0.535 cal/kg
Density at 1 atm and 25C	1.91855 g/L

As a chemical compound, DME is considered relatively stable with reactions or decomposition occurring at severe conditions. In this regard, the decomposition rate of DME is estimated at 1% per year when subjected to a temperature of 493K.

Another chemical property that defines DME is that is a powerful solvent with high solubility for both polar and non-polar substances. In this regard, 1 volume of water takes up 37 volumes of DME. It is also soluble I ether, ethyl alcohol, acetone and chloroform ("Dimethyl ether", n.d.).

3.4. Handling, Safety and Storage

There are various hazard identifiers used to define DME. In the US, the National Fire Protection Association's codes and standards, NFPA 704, categorizes the gas at a flammability of 4 (NFPA, 2021). This means that the gas is extremely flammable with an ability to vaporize completely at ambient environmental conditions (NOAA Office of Response and Restoration, n.d.). The gas' hazard identification information is presented in the following table.

Table 4: DME Identifiers

Category	Designation
DME CAS no.	115-10-06
NFPA Flammability no.	4
NFPA Health no.	2
NFPA stability no.	1

Exposure to the gas has several health effects including frostbites when exposed to the skin, pain and redness when exposed to the eyes, and sore throat, drowsiness, loss of consciousness, and headaches when inhaled ("ICSC 0454 -DIMETHYL ETHER", n.d.). The following table summarizes the health hazards related to exposure to DME.

Table 5: DME Health Hazards

Exposure	Symptom
Inhalation	Headaches, sore throat, drowsiness and loss of consciousness
Skin	Frostbites
Eyes	Blurry vision, pain and redness

The following sections describe the various safety and handling procedures pertinent to DME.

3.4.1. Handling and Storage

Based on the hazardous nature of DME, there are various recommended protocols on how to handle and store the gas. The handling of DME encompasses a variety of personal precautions

such as the wearing and usage of protective gear as well as an intricate understanding of emergency procedures pertinent to the gas. These precautions include; the wearing of self-contained breathing apparatus when in contaminated areas, constant monitoring of oxygen levels and supply within production of contaminated areas ("Safety Data Sheet -DME", 2018), and only allowing trained personnel to respond to uncontrolled leakages. An additional precaution is the use of Personal Protective Equipment PPE of a grade B minimum encompassing; fire-retardant clothing, mechanical resistant gloves and self-contained breathing apparatus ("ICSC 0454 -DIMETHYL ETHER", n.d.). Finally, the lower explosive limit (LEL) should be 10% for the combustible gas ("Safety Data Sheet -DME", 2018).

There are also a variety of measures that should be adopted to handle and store the equipment used in the process of manufacturing and using DME. The most important measures in this regard include, constant inspection of gas cylinders to ensure no damage, not tampering with pressure relief devices in valves and cylinders ("Safety Data Sheet -DME", 2018), and storing gas containers in a cool, well-ventilated and dry area away from direct sources of heat. Additionally, the temperature in the storage area should be limited to a maximum of 52°C (or 125°F), the gas containers for DME should be stored in an upright, well-fastened position, and there should be segregation of full and empty containers. Finally, the cylinders containing DME should be kept at least 20 ft from any heat source.

3.4.2. Safety

As an alternative fuel source, DME exhibits a better safety proposition than other synthetic fuels, because it is a circular hydrogen carrier, meaning it utilizes hydrogen to store energy in a vector form (Styring et al., 2021). DME is synthesized using different methods and

from varying sources, which means that each of its synthesis processes have different safety ratings.

Generally, the synthesis of DME using direct synthesis has lower risk potential, than using indirect synthesis because of the additional processes involved in the latter (De Falco, n.d.). In this regard, the direct synthesis of DME bypasses the synthesis of methanol. Indirect synthesis of DME on the other hand, involves the synthesis of methanol from shale/natural gas. Because methanol is categorized as a category 2 flammable liquid and category 3 toxic substance (De Falco, n.d.), safety precautions have to be put in place when using the indirect method for the synthesis of DME.

The safety risks associated with indirect synthesis include risk of fires and exposure to toxins if in contact with the reactants over prolonged periods of time. In this regard, 200 ppm is the permissible exposure limit (PEL) dictated by the Occupational Safety and Health Administration (Yang et al., 2015).

Another safety consideration in the production of DME using indirect synthesis from methanol, is the incorporation of a floating head storage tank (Yang et al., 2012). This tank alleviates the safety concerns associated with the flammability and volatility of methanol and other raw materials.

3.5. Uses of DME

DME has a variety of uses. The most prominent of these include as a refrigerant (R-E170), as a solvent, as a propellant in industrial aerosol products, and finally, for purposes including transportation fuel, domestic use, and power generation.

4. Process Selection

4.1 Market Analysis and Trends

In order to determine our plant capacity, an analysis had to first be conducted to determine how much DME is currently being produced and compare it with the future demand of DME. The current capacity for DME is about 3 million metric tons while the demand is expected to grow by 530,000 tons by 2025 (Fleisch et. al 2012). It is important to note that specific demand data could not be found so we predicted the future demand using previous years' growth as an indicator. After finding the current production, competitors were researched to see how much they were producing. Plant capacities were found ranging from 20,000 metric tons per year (MTPY) to 100,000 MTPY. From these numbers it was deemed that 50,000 MTPY was a reasonable capacity for the plant design. From this capacity, the material balance was able to be calculated, which will be discussed later in this report.

4.2 Reaction Routes to Producing Product

After conducting a literature review, the proposed alternatives were narrowed to: Methanol Dehydration to form DME (alternative 1), DME production using biogas feedstock (alternative 2), and indirect DME production using a natural gas feedstock (alternative 3). These three were specifically chosen due to representing the present and future possibilities of DME while taking into account availability of research to complete the design.

4.3 Process Screening Using Gross Profit Analysis

One of the main goals for the design was to design a system that is profitable. In order to make sure the selected alternative was profitable, a theoretical economic indicator analysis, shown in equation 1, had to be completed to ensure profitability.

$$\text{Products} * \text{Price} - \text{Reactants} * \text{Price} \quad (6)$$

If the difference came out to be negative then the calculated alternative would not be profitable, but rather cause debt. If the difference was positive then the given alternative would be profitable, thus being a good choice to start a design around.

4.4 Process Comparison and Selection

For the process comparison and selection, each alternative was compared on the basis of economics, impact on the environment, potential location, and safety. Each team member rated the category on a scale of 1-5 based on the literature review and discussed aspects of each alternative. The following chart shows how each alternative scored in each category.

Table 6: Process Comparison and Selection

Considerations:	Alternative 1	Alternative 2	Alternative 3	Weight, %
Economics	18	10	12	40
Environment	13	16	20	25
Location	14	13	9	25
Safety	13	13	16	10
Total	<u>15.25</u>	12.5	13.65	100

As shown in Table 6, the alternative with the highest score was methanol dehydration to form DME. The chemical formula can be seen below and was used to conduct the theoretical economic indicator analysis.

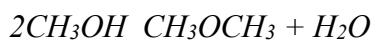


Table 7: Theoretical Economic Indicator for Methanol Dehydration to form DME

	A	B	C
mol	2	1	1
Molecular Weight kg/mol	.03204	.04607	.01802

kg	.06408	.04607	.01802
kg/kg DME	1.39	1	.391
cents/kg	\$0.36	\$0.71	0

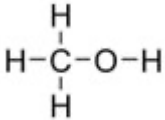
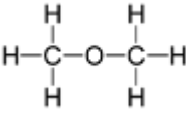
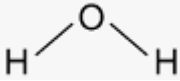
Shown in Table 7 is the preliminary economic analysis that was conducted to ensure that the chosen alternative would be profitable. A represents methanol, B is DME, and C is water. After utilizing equation 6 the theoretical indicator was found to be \$0.21cents/kg DME or \$210/MT DME.

5. Process Description

5.1 Process Chemistry

The irreversible chemical equation for methanol dehydration, equation 1, shows that for every two moles of methanol, one mole of DME and water is produced. The chemical conditions for each component used in the process is show in Table 8.

Table 8: Chemical Conditions for Components

Conditions	Components		
	<i>Methanol</i>	<i>Dimethyl Ether</i>	<i>Water</i>
<i>Molecular Weight</i>	32.04 g/mol	46.07 g/mol	18.02 g/mol
<i>Chemical Formula</i>	CH ₃ OH	CH ₃ OCH ₃	H ₂ O
<i>Chemical Structure</i>			
<i>Boiling Point</i>	64.70°C	-24°C	100°C
<i>Melting Point</i>	-94.60°C	-141°C	0°C
<i>Flash Point</i>	9.7°C	-41.1°C	-
<i>Density</i>	0.79 g/cm ³	1.97 g/cm ³	1 g/cm ³

The mole balance and rate law equations are shown in Table 9. F is defined as flow rate, while W, represents catalyst weight. The rate law equations also show the relationship between

the reactants and products. Methanol dehydration is favored at lower temperatures because it is an exothermic reaction. Therefore, a tubular packed bed reactor is used due to its low operating cost, high conversion per unit mass of catalyst, and ideal for catalytic processes with low temperatures. Maintaining a low temperature is critical to reduce the formation of by-products such as ethylene, carbon monoxide, hydrogen, and coke.

Table 9: Kinetic Rate Equations

Species	Mole Balance Equation	Initial Flow Rate	Rate Laws
<i>Methanol</i>	$dF_{\text{CH}_3\text{OH}}/dW = r'_{\text{CH}_3\text{OH}}$	$F_{\text{CH}_3\text{OH}}(0) = 274$ kmol/hr	$r'_{\text{CH}_3\text{OH}} = -k_1 C_{\text{CH}_3\text{OH}}^2$
<i>Dimethyl Ether</i>	$dF_{\text{CH}_3\text{OCH}_3}/dW = r'_{\text{CH}_3\text{OCH}_3}$	$F_{\text{CH}_3\text{OCH}_3}(0) = 0$	$r'_{\text{CH}_3\text{OCH}_3} = -2r_{\text{CH}_3\text{OH}}$
<i>Water</i>	$dF_{\text{H}_2\text{O}}/dW = r'_{\text{H}_2\text{O}}$	$F_{\text{H}_2\text{O}}(0) = 0$	$r'_{\text{H}_2\text{O}} = -2r_{\text{CH}_3\text{OH}}$

5.2 Process Flow Diagram and Process Description

The dimethyl ether process receives pure liquid methanol from a pipeline, it is then pumped into a mixer and mixes with the recycled liquid methanol. This methanol mixer is then pumped into a vaporizer where it will change phases from liquid to vapor. This vapor methanol mixer continues into a heater that heats up the combined vapor stream to the desired reactor inlet temperature. The effluent from the furnace is fed to the catalytic packed bed reactor. In the reactor, the methanol is being dehydrated by a gamma alumina catalyst and converted into DME and Water. The reactor operates at 90% conversion and the tubes are packed with $\gamma\text{-Al}_2\text{O}_3$. The product from the reactor is then cooled and sent to the first distillation column where the DME separation occurs. The overhead product is the desired DME product which is stored in a tank

between a 7 through 14 bar and up to 52°C. The bottoms products are, now in the liquid phase, methanol and water which are sent to a second distillation column for further separation. The second distillation overhead product is methanol which will be recycled back into the system and the bottoms product is wastewater which will be sent to SNF Holding Company Plaquemine treatment facility. Wastewater treatment will reduce pollutants in water and negative health effects on life species.

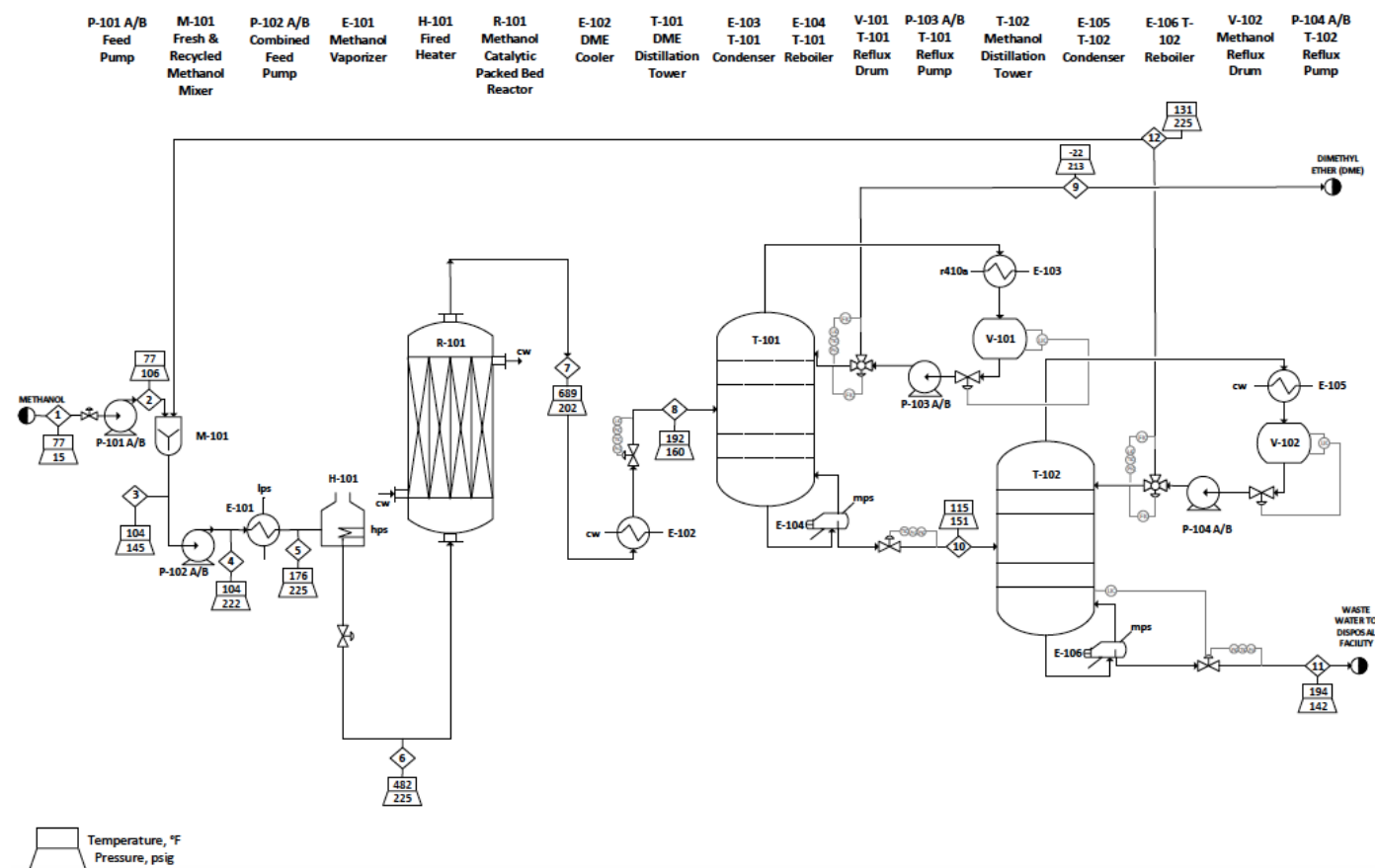


Figure 2: Production of Dimethyl Ether Process Flow Diagram

6. Material and Energy Balances

6.1 Material Balances

As previously mentioned, the basis of calculation was determined to be 50,000 MTPY of DME.

From this number, the overall material balance was able to be calculated using the stoichiometric ratio of the reaction. The capacity was first taken from a yearly time period to 152 MTPD. This number was then converted into a mass flow rate and then to a molar flow rate. After applying the stoichiometric ratio, the wastewater flow rate and feed flow rate were calculated. In order to complete the individual unit balances, assumptions about the molar compositions were made (Diemer et. al 2010).

Block Flow Diagram Material Balance

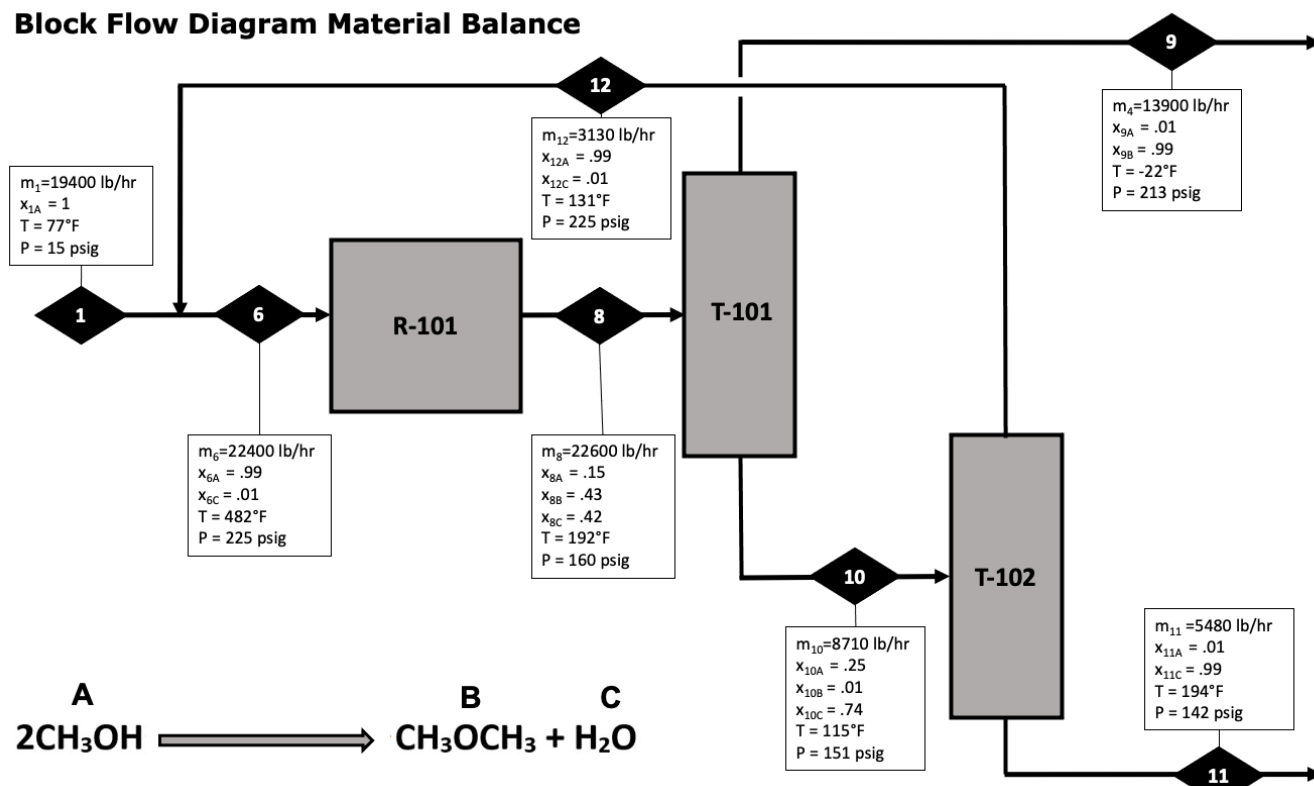


Figure 3: Material Balance for Design

Figure 3 shows the total material balance for each process stream. Using the assumed molar compositions and the degree of freedom (DOF) analysis, the individual stream flowrates were able to be calculated.

6.2 Energy Balances

In order to complete the energy balance around the reactor, temperature, flowrates, and specific heat capacities were needed, as shown in Equation 7. The temperature for the reactor was determined based off the literature review and the specific heat capacity was calculated at ambient temperature. Since the streams were mixed, the molar compositions were used to determine the specific heat capacity for each component in the stream. The individual heat capacities were then added to get the total heat capacity for the stream.

$$\sum mC_pT_2 = \sum mC_pT_3 \quad (7)$$

In order to calculate the total energy balance, the process was simulated in ASPEN. Using the degree of freedom (DOF) analysis, the ASPEN simulation was simulated vessel by vessel. First, the reactor was converged by defining the temperatures and pressures for each stream and only defining the molar composition and molar flow for the input streams. After checking to see if the output values matched the calculated values in Figure 3, a separator was added to the simulation. Since the input stream for the first distillation column was calculated by Aspen, the composition and molar flow rate for the bottoms stream was only defined. Once the simulation ran again, it was proved that the molar flow rate and compositions Aspen calculated for the first overhead stream also matched the calculations in Figure 3. Lastly, the same steps were followed for the last distillation column until a fully converged simulation which molar flows and compositions for each stream matched the material balance that is shown in Figure 3. The recycle stream is split into two streams to make it easier to converge and more accurate. Each stream converged

and the simulated energy balance for the reactor was compared with the calculated energy balance to check accuracy. Since all values were within a 5% error, the simulation was deemed correct and the total energy balance can be seen in Figure 3. The simulated ASPEN is shown in Figure 3 and the energy balance values can be seen in Table 10.

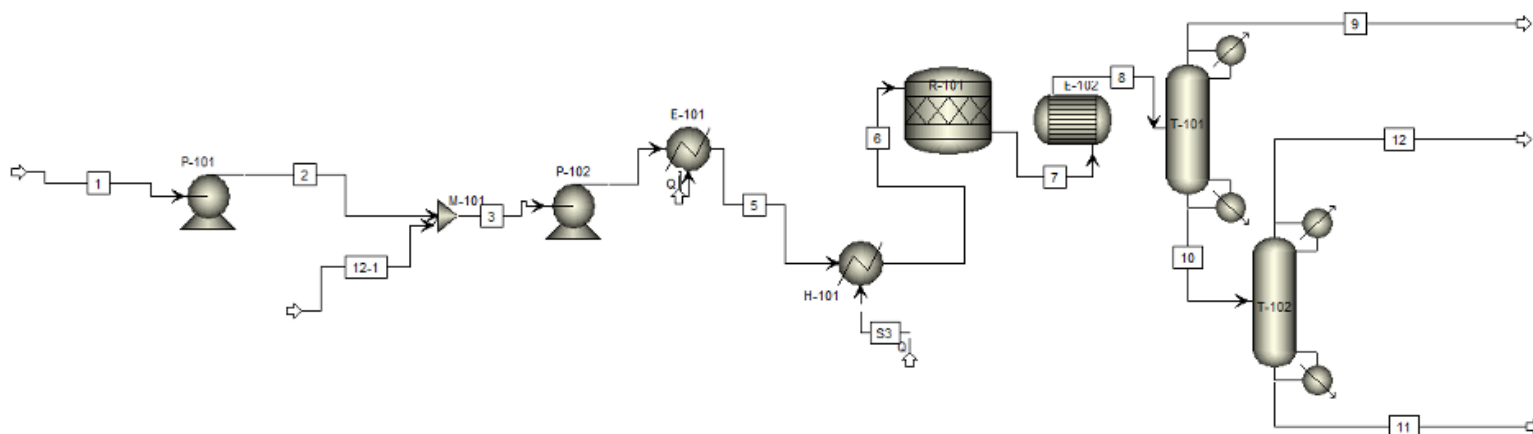


Table 10. Energy Balance Calculations

Methanol Dehydration R-101	
Temperature	689°F
R-101 Duty	-1.36×10^7 BTU/hr
E-101 Duty	9.67×10^6 BTU/hr
H-101 Duty	5.40×10^6 BTU/hr
E-102 Duty	-1.14×10^7 BTU/hr

DME Distillation T-101	
Temperature	86°F/114.8°F
E-103 Duty	-3.39 × 10 ⁶ BTU/hr
E-104 Duty	2.36 × 10 ⁶ BTU/hr

Methanol Distillation T-102	
Temperature	158°F/194°F
E-105 Duty	-1.18 × 10 ⁷ BTU/hr
E-106 Duty	1.14 × 10 ⁷ BTU/hr

7. Utilities

To carry out the production of DME, power, steam, cooling water, wastewater disposal, and refrigerants were all considered. Table 11 summarizes the necessary utility requirements for each piece of major equipment.

Table 11. Summary of Utilities

Power kWh/y	
P-101 A/B	56900
P-102 A/B	75800
P-103 A/B	41100
P-104 A/B	7900
Steam kg/y	
E-101 (lps)	193000
H-101 (hps)	50000
E-104 (mps)	10000
E-106 (mps)	49000
Cooling Water m ³ /y	
R-101	104000
E-102	149000
E-105	29100
Wastewater Disposal m ³ /y	
T-102	19900
Refrigerant r140a GJ/y	
E-103	432

8. Equipment List and Description

8.1 P-101

This pump is responsible for increasing and regulating the initial pressure of methanol before it is delivered the system. The pump increases the pressure of fresh methanol from 1 bar to 7.3 bar, before it is fed to the vaporizer.

8.2 P-102

This pump is responsible for increasing and regulating the pressure of the combined stream of methanol after it leaves the mixer. The pump increases the pressure of fresh methanol from 10.0 bar to 15.2 bar, before it is fed to the vaporizer.

8.3 E-101

This is a vaporizer that takes methanol from a liquid to a gaseous state. It is made of carbon steel and has a cross-sectional area of 1.02 m^2 . The vaporizer has a heat transfer area of 56.3 m^2 and a duty of $1.02 \times 10^7 \text{ kJ/hr}$.

8.4 H-101

The third component in the process flow is a furnace that is responsible for heating methanol to the idealized temperature of 250°C before it is fed to the reactor. The furnace is constructed using carbon steel to withstand high temperature. It has a maximum pressure rating of 45 bar and a duty of $5.7 \times 10^6 \text{ kJ/hr}$.

8.5 R-101

This is a catalytic packed bed reactor. There are 34 tubes each comprised of 733.03 kg of $\gamma\text{-Al}_2\text{O}_3$ catalyst and as the methanol passes through the tubes it is dehydrated to form DME and water. Each tube has a diameter of .03m while the reactor has a diameter of 1.33 meters and an overall height of 4.48 meters. The construction of the tower section of the reactor comprises mild carbon steel (A516 grade), whereas the tubing is made of stainless steel (grade 316). This reaction is exothermic and if the temperature gets too high, the process will begin to form byproducts and

the catalyst will deactivate. To prevent this, cooling water is passed through the shell side of the reactor to maintain the desired temperature. Its maximum pressure rating is 15 bar.

8.6 E-102

This is a shell and tube heat exchanger made of carbon steel. It acts as a cooler lowering the temperature of the mixture leaving the reactor. The heat exchanger cools DME/water/methanol mixture from 365°C to 89°C before it is fed to the first distillation column which is responsible for separating DME from the mixture. The maximum pressure rating of the heat exchanger is 14 bar. It comprises a floating-head shell and tube design with the main construction material being carbon steel.

8.7 T-101

This is a tray-type distillation column with 22 valve trays, a reboiler and a condenser. The average tray spacing is .61m, and the column is responsible for the separation of DME from a water/methanol mixture. It is predominantly made of carbon steel, with an overall height of 16m and a diameter of 12m. The feed for the column contains DME, water and methanol. The distillate on the other hand comprises of DME whereas water and methanol mixture is collected at the bottom. The maximum pressure rating for the column is 15 bar.

8.8 T-102

This is a tray-type distillation column with 15 valve trays, a reboiler and a condenser. The average spacing between the trays is .8m. The column is responsible for the separation of methanol that goes into the recycling stream from waste water. It is predominantly made of carbon steel,

with an overall height of 20m and a diameter of 13m. The feed for the column contains traces of DME, water and methanol. The distillate on the other hand comprises of methanol whereas water is collected at the bottom. The maximum pressure rating for the column is 15 bar.

9. Specification Sheets

9.1 P-101A/B Specifications

Pump				
Identification:	Item:	Pump		
	Item No:	P-101	Date	2/23/2022
	No. Required	2		
	C _{TPI} (\$)			
Function:	Pump liquid methanol from 1 bar to 15.2 bar			
Operation	Continuous			
	Inlet	Outlet		
Materials Handled				
Mass Flow(kg/hr)	8778	8778		
Mole flow (kgmol/hr)	274	274		
Component Flow (kgmol/hr):				
Dimethyl Ether	0	0		
Methanol	274	274		
Water	0	0		
Temperature (C)	25	25		
Pressure (bar):	1	15.5		
Vapor Fraction:	0.0	0		
Design Data:				
Power (kW)	7.2	Material:	Carbon Steel – A36	
Efficiency (%)	60	Type:	Centrifugal	
ΔP	6.3			
Utilities:				

Comments:	
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9.2 P-102A/B Specifications

Pump				
Identification:	Item:	Pump		
	Item No:	P-102	Date	2/23/2022
	No. Required	2		
	C _{TPI} (\$)			
Function:	Pump liquid methanol from 10 bar to 15.2 bar			
Operation	Continuous			
	Inlet	Outlet		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (kgmol/hr):				
Dimethyl Ether	0	0		
Methanol	315	315		
Water	3.18	3.18		
Temperature (C)	40	40		
Pressure (bar):	10	15.2		
Vapor Fraction:	0.0	0		
Design Data:				
Power (kW)	9.6	Material:	Carbon Steel – A36	
Efficiency (%)	60	Type:	Centrifugal	
ΔP	5.2			
Utilities:				
Comments:				

9.2 E-101 Specifications

Vaporizer

Identification:	Item:	Vaporizer		
	Item No:	M-101	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Vaporization of liquid methanol			
Operation	Continuous			
	In	Out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (kgmol/hr):				
Dimethyl Ether	0.0	0.0		
Methanol	315	315		
Water	3.18	3.18		
Temperature (C)	40	80		
Pressure (bar):	15.2	15.5		
Vapor Fraction:	0.0	1.0		
Design Data:				
Cross-sectional area	1.02 m ²	Material:	Carbon Steel	
Diameter	1.14 m			
Duty (Q) kJ/hr	1.02 * 10 ⁷			
Heat transfer area	56.3 m ²			
Maximum Pressure rating	15 bar			
Utilities:	Low Pressure Steam 4.5 bar = 24160 kg/hr			
Comments:				

9.3 H-101 Specifications

Electric Furnace				
Identification:	Item:	Electric Furnace		
	Item No:		Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Heat stream to 250°C			

Operation	Continuous			
	In	Out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (Kmol/hr):				
Dimethyl Ether	0	0		
Methanol	315	315		
Water	3.18	3.18		
Temperature (C)	80	250		
Pressure (bar):	15.5	15.5		
Vapor Fraction:	1	1		
Design Data:				
Superheated Temperature (C)	400	Material:	Carbon Steel	
Duty (Q) kJ/hr	$5.7 * 10^6$			
Maximum Pressure rating	45 bar			
Utilities:	hps = 6255 kg/hr			
Comments:				

9.4 R-101 Specifications

Reactor				
Identification:	Item:	Catalytic Packed Bed Reactor		
	Item No:	R-101	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Dehydration of methanol to produce DME and water			
Operation	Continuous			
	In	Out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (Kmol/hr):				
Dimethyl Ether	0	136.92		
Methanol	315.25	47.76		

Water	3.18	133.74		
Temperature (C)	250	365		
Pressure (bar):	15.5	13.9		
Vapor Fraction:	1.0	1.0		
Design Data:				
Diameter (m)	1.33	Material:	Carbon Steel	
Overall height (m)	4.48			
Number of Tubes	34	Area (m ²)	12.41	
Maximum Pressure rating	15 bar			
Combined Tube Volume m ³	19			
Utilities:	CW	12951.38 kg/hr		
Comments:	Temperature maintained by cooling water Catalyst in tubes is γ -Al ₂ O ₃ Total catalyst weight is 24923 kg			

9.5 E-102 Specifications

Reactor Effluent Cooler				
Identification:	Item:	Shell and Tube Heat Exchanger		
	Item No:	E-102	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	To cool the DME stream coming from the reactor to 89°C			
Operation	Continuous			
	Hot in	Hot out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (Kmol/hr):				
Dimethyl Ether	136.92	136.92		
Methanol	47.76	47.76		
Water	133.74	133.74		
Temperature (C)	365	89		

Pressure (bar):	13.9	10.4		
Vapor Fraction:	1.0	1.0		
Design Data:				
Q (kJ/h)	1.2×10^7	Material:	Carbon Steel	
A (m ²)	101.8			
Maximum Pressure rating	14 bar			
Utilities:	cw	18566.41 kg/h	T _{in} = 30°C T _{out} = 45°C	
Comments:	Process stream in shell (DME/methanol/water)			

9.6 T-101 Specifications

1 st Distillation Column				
Identification:	Item:	DME Separator		
	Item No:	T-101	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Separate DME from methanol/water			
Operation	Continuous			
	Feed	Liquid Distillate	Liquid Bottoms	
Materials Handled	Methanol/DME/Water	Methanol/DME	Methanol/Water	
Mass Flow(kg/hr)	10245.83	6292.36	3952.83	
Mole flow (kgmol/hr)	318.43	137	181.4	
Component Flow (kgmol/hr):				
Dimethyl Ether	136.92	135.63	1.81	
Methanol	47.76	1.37	45.35	
Water	133.74	0.00	134.24	
Temperature (C)	89	-30	46	
Pressure (bar):	11	14.7	10.4	
Vapor Fraction:	1	0.0	0.0	

Design Data:					
Reflux ratio	1.7	Material:	Carbon Steel		
Number of actual trays	22				
Tray Spacing (m)	1				
Total tower height (m)	16				
Column diameter (m)	.8				
Maximum Pressure rating	15 bar				
Associated Component					
Condenser (E-103)	refrigerant : 432 GJ/y	A = 100.6 m ²	Q = 3.58x10 ⁶ kJ/hr	Fixed head, carbon steel	Max pressure = 10bar
Reboiler (E-104)	mps: 1256 kg/hr	A = 22m ²	Q = 2.49x10 ⁶ kJ/hr	Floating head, carbon steel	Max pressure = 11bar
Reflux Drum (V-101)	L = 2.89m	D = 1.14m	Carbon Steel	Max pressure = 10.3 bar	
Reflux Pump (P-103 A/B)	Power = 5.2 kW	Efficiency = 40%	$\Delta P = 4.6\text{bar}$	Centrifugal/Carbon Steel	
Utilities:					
Comments:					

9.7 T-102 Specifications

2 nd Distillation Column				
Identification:	Item:	Methanol Separator		
	Item No:	T-102	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Separate methanol from water			
Operation	Continuous			
	Feed	Liquid Distillate	Liquid Bottoms	
Materials Handled				
Mass Flow(kg/hr)	3952.83	1417.3	2485.26	
Mole flow (kgmol/hr)	181.4	44.43	137	

--- (Contd)

Component Flow (kgmol/hr):					
Dimethyl Ether	1.81	0.00	0.00		
Methanol	45.35	43.99	1.37		
Water	134.24	.44	135.63		
Temperature (C)	46	55	90		
Pressure (bar):	10.4	15.5	9.8		
Vapor Fraction:	0.0	1.0	0.0		
Design Data:					
Reflux ratio	4.472	Material:	Carbon Steel		
Number of actual trays	15				
Tray spacing (m)	1				
Total tower height (m)	20				
Column diameter (m)	1.16				
Maximum Pressure rating	15 bar				
Associated Components					
Condenser (E-105)	cw: 294250 kg/hr	A = 22.7 m ²	Q = 1.24x10 ⁷ kJ/hr	Floating head, carbon steel	Max pressure = 7 bar
Reboiler (E-106)	mps: 6130 kg/hr	A = 83.0 m ²	Q = 1.20x10 ⁷ kJ/hr	Floating head, carbon steel	Max pressure = 11 bar
Reflux Drum (V-102)	L= 2.53m	D = .85m	Carbon steel	Max pressure 7.3 bar	
Reflux Pump (P-104 A/B)	Power = 1.0 kW	Efficiency = 40%	ΔP = 4.1bar	Centrifugal/Carbon Steel	
Utilities:					
Comments:					

10. Equipment Costs and Capital Investment

To determine the various equipment costs, a modified version of CAPCOST software was applied on Microsoft Excel. In this regard, the software used properties such as vessel sizing and construction material to determine the estimated costs of various equipment throughout the process flow. The Chemical Engineering Plant Cost Index (CEPCI) was then used to adjust the realized estimates for inflation to the current year. Using CAPCOST, the purchased equipment costs and bare module costs were realized and summarized in Table 11 as shown below.

Table 12. Summary of Equipment Costs Using CAPCOST

			<u>Unit Number</u>	100				
			<u>CEPCI</u>	710				
User Added Equipment								
Evaporators	Type	Area (square meters)	Pressure (barg)	MOC	Volume (cubic meters)		Purchased Equipment Cost	Bare Module Cost
K-101	Vessel with Internal Coil		20	Carbon Steel	16.6		\$65,100	\$284,000
Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)		MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost
E-101	Floating Head	85	16.7		Stainless Steel / Carbon Steel	118	\$34,300	\$194,000
E-102	Fixed, Sheet, or U-Tube	13.7	12		Stainless Steel / Carbon Steel	101	\$42,200	\$201,000
E-103	Floating Head	13.4	13.2		Stainless Steel / Carbon Steel	22	\$32,700	\$155,000
E-104	Floating Head	18.6	8.4		Stainless Steel / Carbon Steel	22.7	\$32,800	\$158,000
E-105	Floating Head	8.88	13.2		Stainless Steel / Carbon Steel	83	\$42,100	\$199,000
E-106	Fixed, Sheet, or U-Tube	12.4	16.6		Stainless Steel / Carbon Steel	12.4	\$27,600	\$133,000

Fired Heaters	Type	Heat Duty (MJ/h)	Steam Superheat (°C)	MOC	Pressure (barg)		Purchased Equipment Cost	Bare Module Cost
H-101	Process Heater	5070		Carbon Steel	54		\$868,000	\$1,990,000
Pumps (with drives)	Pump Type	Power (kilowatts)	# Spares	MOC	Discharge Pressure (barg)		Purchased Equipment Cost	Bare Module Cost
P-101	Centrifugal	7.2	1	Carbon Steel	31		\$12,640	\$65,000
P-102	Centrifugal	9.6	1	Carbon Steel	15.2		\$9,810	\$42,700
P-103	Centrifugal	5.2	1	Carbon Steel	11.2		\$11,480	\$46,800
P-104	Centrifugal	1	1	Carbon Steel	8.8		\$8,760	\$34,900
Towers	Tower Description	Height (meters)	Diameter (meters)	Tower MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
T-101	22 Stainless Steel Valve Trays	16	0.8	Carbon Steel		18	\$82,600	\$220,000
T-102	10 Stainless Steel Valve Trays	20	1.16	Carbon Steel		18	\$73,600	\$309,000
Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
V-101	Vertical	2.89	1.14	Carbon Steel		12.4	\$9,640	\$55,700
V-102	Vertical	2.53	0.85	Carbon Steel		8.8	\$6,650	\$30,500
						Total Purchased		\$1,359,980

----- Contd.

						Equipment Cost		
						Total Adjusted 10%		\$1,495,978
Catalyst		Weight (Kg)	Unit Cost	Units	Cost			Total Cost
γ -Al ₂ O ₃		24523	207.4	24523				\$5,086,070.20
Project Estimate								Total
Project Estimate								\$6,582,048.20

The realized costs were then adjusted using a 10-percent margin of error to accommodate any additional equipment that may have been overlooked. From the table above the final project estimate was determined to be \$6,583,797.20.

11. ASPEN Simulation of Process

As shown in Figure 4, the process was simulated using ASPEN Plus. In order to ensure that the system converged, a step-by-step design was implemented. What this means is that each piece of equipment was individually placed and converged before moving to the next piece of equipment. By having each piece of equipment converge, the overall design was able to converge once all equipment was simulated.

12. Economic Evaluation

An overview of the economic analysis can be seen in Table 13 below.

Table 13. Economic Summary

Economic Evaluation	
Total Capital Investment, 10^6	\$10.2
Annual Total Production Costs, 10^6	\$34
Annual Sales, 10^6	\$37
Payback Period, yrs	4.2
Return on Investment, %/year	22
Discounted Cash Flow Rate of Return, %/yr	13
Net Present Value, 10^6	\$8
Salvage Value, 10^6	\$1
Cumulative profit, 10^6	\$23

Figure 5 shows the cash flow diagram for the system. It is important to note that the values represented already take into account the total production costs. As seen, in year 13, profit turns back negative. This is due to an assumed 2% inflation rate for total production costs coupled with the depreciation of equipment.

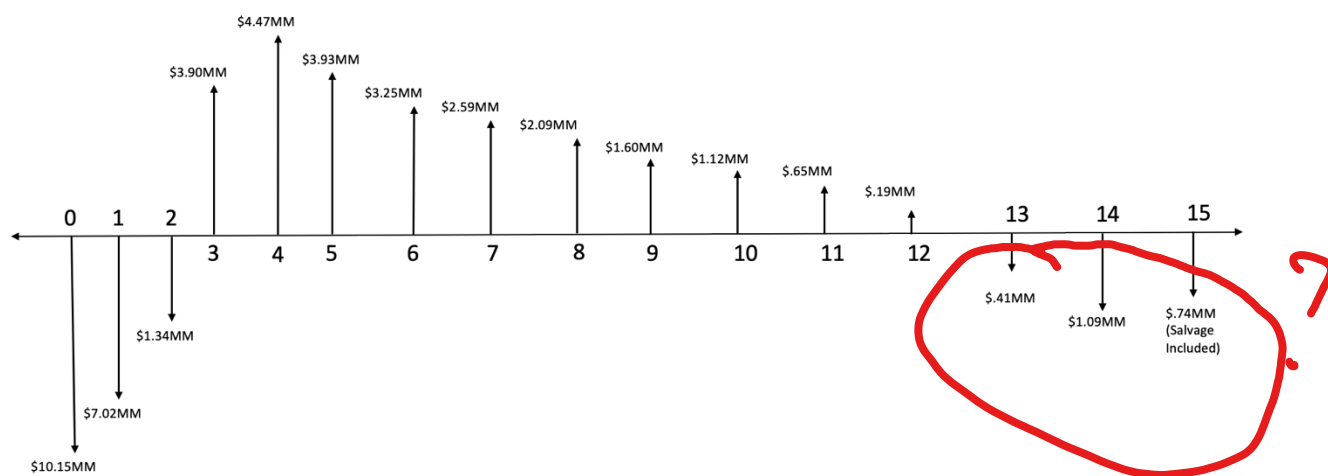


Figure 5. Cash Flow Diagram

13. Safety and HAZOP Analysis

Safety plays a crucial role in the success of the project. A hazard and operability (HAZOP) analysis presents a means of assessing how various components within the plant may deviate from their normal operations and pose safety and health risks to personnel, and how to mitigate these deviations. For this project, a HAZOP analysis was conducted for the second distillation column, the methanol tower, which is responsible for the separation of methanol for recycling from water/methanol mixture.

The methanol tower is a distillation column comprising of a feed line, a distillate line and a bottom line. It is a crucial component in the proposed plant for the synthesis of DME from methanol to be established in Plaquemine, Louisiana.

The general Guidelines for Safety Guidelines in Accordance with Rules and Regulations of Plaquemine, Louisiana are as follows (Ayres, 2016):

I. Pre Line Opening Job Preparations –

- The shutting down and energy isolation of all process systems prior to any line opening involving process piping, equipment or vessels (4.1.1).
- The draining and/or depressurization of all process piping, equipment or vessels to ensure clearance of hazardous materials (4.1.2).
- Ensuring temperatures for the process piping, equipment or vessels have sufficiently cooled to allow for safe work (4.1.3).

II. Line Opening Job Planning –

- The barricading of affected areas with a minimum of 10 ft radius as a precautionary area (4.2.1.1)
- The issuance of permits strictly by authorized personnel (4.2.2.1)

With the above guidelines the project involved a maximum exposure of 200 ppm from methanol. In addition, the general guidelines adopted by the City of Plaquemine where the proposed plant is expected to be established, the HAZOP analysis for the second distillation which constitutes the methanol tower can be conducted as follows.

I. T-102 Feed Line – Entry of reactants (methanol/water mixture) into the distillation column.

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the feed line	There is pressure build up in the feed line leading into the tower	- Blockage in the system	- Failure of feed line tube - Risk of expansion of column and bursting	Installation of quick-pressure relief valves at strategic locations before and after the column.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in feed line	There are sudden pressure losses in the streams leading to the column	- Leakages in the system	- Insufficient reactant material entering the column	Pressure alarms at the feed, distillate and bottom streams	- Installation of pressure gauge - Checking maintenance schedule and procedures
3	Flow	Reverse	Backflow from T-102	The contents of the tower flow back to the feed line	- Clogging and blockages within the tower	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow- Following the stipulated maintenance schedule and procedures
4	Temperature	More	Increase in feed temperature	There is sudden increase in temperature at the feed of T-102	- Clogging of inlet into tower	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at feed entry point. - Panel alarms to warn of high pressure or temperature	- Installation of a temp gauge - Checking maintenance schedule and procedures

II. T-102 Distillate Line – Transportation of recycled methanol from the distillation column back to the mixer.

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the distillate line	There is pressure build up in the distillate line transporting recycled methanol to the mixer	-Blockage in the mixer or further up the distillation line	- Failure of distillate line tube - Risk of expansion of mixer and bursting. - Failure of mixer	Installation of quick-pressure relief valves at strategic locations before the mixer.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in feed line	There are sudden pressure losses in the stream leading to the mixer	- Leakages in the distillate line	- Inefficiencies within the tower leading to less methanol distillate	Pressure alarms at the exit of the column where the distillate line begins.	- Installation of pressure gauge - Checking maintenance schedule and procedures
3	Flow	Reverse	Backflow to T-102	The contents of the distillate line flow back to the tower	- Clogging and blockages within the line	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow- Following the stipulated maintenance schedule and procedures
4	Temperature	More	Increase in distillate line temperature	There is sudden increase in temperature at distillate line transporting recycled methanol	- Clogging of inlet into the mixer	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at mixer entry point. - Panel alarms to warn of high pressure or temperature	-Installation of a temp gauge - Checking maintenance schedule and procedures

III. T-103 Bottom Line – Transportation of wastewater from the distillation column to treatment plant.

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the bottom line	There is pressure build up in the bottom-line transporting wastewater to treatment plant	-Blockages within bottom line	- Failure of bottom-line tube - Risk of expansion and bursting of the line.	Installation of quick-pressure relief valves at strategic locations within the line.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in bottom line	There are sudden pressure losses in the stream within the bottom line leading away from the tower	- Leakages in the bottom line	- Inefficiencies within the tower causing decreased flow of wastewater from the tower	Pressure alarms at the exit point from the tower joining the bottom line	- Installation of pressure gauge - Checking maintenance schedule and procedures
3	Flow	Reverse	Backflow to T-102	The contents of the bottom line flow back to the tower	- Clogging and blockages within the line	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow- Following the stipulated maintenance schedule and procedures
4	Temperature	More	Increase in bottom line temperature	There is sudden increase in temperature at bottom line transporting wastewater to the treatment plant	- Clogging of the line at various points	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at exit point of the tower to the bottom line. - Panel alarms to warn of high pressure or temperature	-Installation of a temp gauge - Checking maintenance schedule and procedures

14. Discussion

Over the course of completing the design, there were assumptions made for the molar compositions of the process streams and for the heat exchanger duties. These values were obtained through literature reviews. As mentioned, the energy balance was assumed to be correct from ASPEN Plus due to similar results being obtained for the reactor energy balance. The economic analysis was assumed to be over a 15 year life span, and a 2% inflation rate was assumed. It is also important to note that for calculation purposes, 8,000 on stream hours was used. Moreover, the median salary for an operator in Plaquemine is \$59,029 (Glassdoor 2022). As a result, we generously set our operator salary at \$70,000 per year and determined that we need three operators per shift and three shifts per day.

not

clear

15. Conclusion and Recommendations

Overall, 50,000 MTPY of DME is being produced at 99.9% purity. This system would be in operation for 329 days out of the year (90% utilization). It is recommended to not produce more than that due to the still emerging market for DME. It has not yet been discovered how to solely rely on DME for transportation fuel, so the market is currently limited. The selected process of methanol dehydration allows for pure methanol to be imported via pipeline and reacted to form DME. Specifically for this design, it is recommended to salvage after year 12 to prevent the negative losses in years 13-15. However, with the present salvage at year 15, the overall profit is \$23MM with a 22% return on investment. As a result of this, it is recommended to continue with the design of this plant. Further analysis on E-102 is also recommended due to the drastic drop in temperature. There may be an additional opportunity for energy savings by recovering the lost heat.

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17. Appendix

Direct Costs	
Purchased equipment, E'	1.496
Delivery, fraction of E'	0.150
Subtotal: delivered equipment	1.646
Purchased equipment installation	0.773
Instrumentation&Controls(installed)	0.592
Piping (installed)	1.119
Electrical systems (installed)	0.181
Buildings (including services)	0.296
Yard improvements	0.165
Service facilities (installed)	1.152
Total direct costs	5.924
Indirect Costs	
Engineering and supervision	0.543
Construction expenses	0.675
Legal expenses	0.066
Contractor's fee	0.362
Contingency	0.724
Total indirect costs	2.370
Fixed capital investment (FCI)	8.294
Working capital (WC)	1.465
Total capital investment (TCI)	9.758

Figure 6. Direct and Indirect Costs

AVERAGE

Average Student Original Graded Assignment for Final Project Report

TWO- STEP PRODUCTION OF 1,3 BUTADIENE FROM ETHANOL

Senior Design & Professionalism II Final Report

Submitted by:

Mohamed Akinotocho
Cayla Alexander
Duaa Al Badri
Jeavun Christie
Au'Myia Collins

83%

To:

Dr. Emmanuel Dasa
Senior Design Instructor

Department of Chemical Engineering
College of Engineering
Prairie View A&M University

April 29, 2022

Abstract:

A plant utilizing a two-step process, which takes a 95% ethanol stream (by mass) and produces a 98% 1,3-butadiene stream, was designed for this project. The production goal of this plant was 200,000 tonnes of butadiene with the main motivation behind the recent rise in butadiene prices behind the project. The process first passes ethanol through a catalytic dehydrogenation reactor to convert ethanol to acetaldehyde and hydrogen. A kinetic model was used to determine the reaction rates and operating conditions of the reactor. The acetaldehyde is further reacted with ethanol in a catalytic reactor to form butadiene. A hydrogen byproduct stream is generated in this design also.

This report provides a design and economic analysis to produce 1,3 butadiene on the Gulf Coast of Texas. Process flow sheets, energy utility requirements, and equipment summaries are provided and analyzed. Process profitability is sensitive to the cost of both ethanol and butadiene. It is shown that the plant is profitable for its expected 12-year lifespan with an expected return on investment of 3% and net present value of \$30,964,090.78. The process becomes unprofitable if the price of ethanol increases overtime. A combination of increased ethanol price and decreased price of butadiene will cause the plant to be unprofitable as well. This plant construction is only recommended given an acceptable price of ethanol and butadiene.

*Low
return*

Letter of Transmittal

College of Engineering Department of Chemical Engineering
Prairie View A&M University - Prairie View, Texas 77446

April 29, 2022

Department of Chemical Engineering

Roy G. Perry College of Engineering

Prairie View A&M University

100 University Dr.

Prairie View, TX 77449

Dear Dr. Emmanuel Dada,

Our group has analyzed a two-step process of converting ethanol to 1, 3-butadiene. Enclosed is our solution to the design problem you proposed. Our plant design involves two reaction sections, both of which use heterogeneous catalysts in shell-and-tube packed bed reactors, and two separation sections to purify the products and recycle the unreacted feed. For the catalyst we used both a copper chromite and tantala-silica heterogeneous catalyst. We have also designed a Dowtherm heating system for our process, which will supply heat to the reactor sections.

This report provides details on the process equipment required and the potential profitability of the plant. The design determined a liquid feed flow rate of 155,000 lb/hr of ethanol and a production rate of 56,000 lb/hr of butadiene. Production was assumed to operate 24 hours a day for 330 days out of the year.

Sincerely,

Mohamed Akinotocho

Cayla Alexander

Duaa Al Badri

Jevaun Christie

Au'Myia Collins

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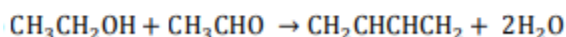
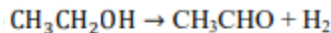
1. Project Scope

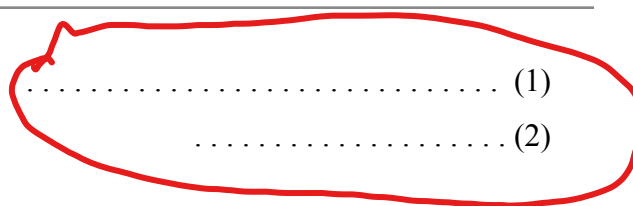
1.1 Problem Statement

Prior to and during World War II, 1,3 butadiene was made from ethanol. The increased growth of the petrochemical industry caused this process to be very uneconomical. The use of ethylene crackers made for an increase in technological changes due to the unwanted increase in cost, limited supply, and growing production of ethanol. The use of the raw material, ethanol, showed better benefits such as reducing the use of fossil fuels by using this renewable feedstock.

The goal of our project is to explore efficient routes in the production of 1,3 butadiene from ethanol. These routes are taken based on economic concerns, safety, environmental impact, and manufacturing factors. With the United States being the world's leading producer of the corn-based biomass, ethanol, using this as our raw material is very convenient. As a group, our primary objective was to establish a process route out of the many that were found through literature research. Choosing our primary process route was required to design our material and energy balances, block flow diagram, and process flow diagram. The price of butadiene has increased from an average of \$0.60/lb prior to the 2011 discovery, to over \$1.60/lb today. The increased pressure of making butadiene has led to the necessity of using other feedstocks.

The 1,3-Butadiene market keeps growing year after year because it is highly used in the manufacturing of synthetic rubbers or elastomers. However the price has been decreasing because the industry has shifted its focus towards developing bio-based alternatives to 1,3 butadiene due to the fact that 1,3 butadiene is a carcinogenic substance. Despite the health issue due to exposure 1,3-butadiene is still a primordial substance, in order to satisfy the demand and take advantage of the long-term price projections for butadiene, while satisfying our own needs we have decided to design a plant to make 271,230 metric tonnes of butadiene per year from ethanol. Our plant will work 330 days/year meaning we will be producing 90.41 % of the time throughout the year, the rest of the days will be used for cleaning and holidays. The current price of butadiene on the market is \$1.01/lb and of ethanol is 27 cents/lb. *maintenance* We have decided to use a two-step process for our production of 1,3-butadiene. The reaction occurs in two steps:





(1) Vapor-phase dehydrogenation of ethanol to acetaldehyde, and (2) the reaction of ethanol and acetaldehyde over a fixed-bed tantalum on silica catalyst to butadiene at 364°C. Optimal conditions for the second step are a 0.6/hr liquid-hourly-space-velocity, and a 2.70:1 molar ratio of ethanol to acetaldehyde. The catalyst must be regenerated by burning off coke at 400°C every 4-5 days, so our plant design must take that into consideration.

Since the team decided to locate the plant in Texas, one important factor to acknowledge in economics is that ethanol price increases adequately during the inter-harvest period. This tends to typically happen 3-4 months throughout the year when sugar cane cannot be harvested and local ethanol plants shut down. In past years, Texas and more states that are based in the south have produced a high percentage of ethanol throughout the years and has also been the main location for its manufacturing. Corn ethanol in the U.S. has no such restriction, as corn can be stored year-round. Which includes a freight cost to the plant site in the cost of ethanol itself.

The plant design should be as environmentally friendly as possible, at a minimum meeting Federal and state emissions regulations. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate.

1.2 Client identification and recognition of need

Prior to and during World War II, butadiene was made from ethanol. The global growth of the petrochemical industry made that route uneconomical. However, with the increase in the cost of, and limited supply of, butadiene from ethylene crackers, and the growing production of ethanol, companies are beginning to consider this technology again. A side benefit is the renewable feedstock, reducing our dependence on fossil fuels. To take advantage of the long-term price projections for butadiene, as well as ensure supply for your own needs, our team has been assembled to design a plant to make 200,000 tons of butadiene per year from ethanol.

1.3 Project goals and objectives

The focus of this report is on the implementation of the Ostromislensky process in a large-scale industrial plant, which now has the potential to be highly profitable due to the increase in butadiene price. However, detailed research on the Ostromislensky process only occurred during the years shortly after World War II, and little research has been done since then. The research that was done was carried out by the Mellon Institute for the Carbide and Carbon Chemicals Corporation, whose limited data was used as the basis for our design (Corson, 1950).

1.4 Contemporary issues and impact of project on society

1.4.1 Contemporary issues relevant to project

Little is known today about the process, other than what was published shortly after World War II. The most successful process was the Ostromislensky process developed and operated by Carbide and Carbon Chemicals Corporation. The reaction occurs in two steps: vapor-phase dehydrogenation of ethanol to acetaldehyde and the reaction of ethanol and acetaldehyde over a fixed-bed Tantalus on silica catalyst to butadiene at 350°C. Optimal conditions for the second step are a 0.6/hr liquid-hourly-space-velocity, and a 2.65:1 molar ratio of ethanol to acetaldehyde. The catalyst must be regenerated by burning off coke at 400°C every 4-5 days, so your plant design must take that into consideration.

1.4.2 Potential impact of project on society

The discovery and exploitation of large quantities of shale gas in the United States has resulted in large shifts in the petrochemical market in the past few years. Copious quantities of inexpensive ethane in shale gas have increased the amount of ethane used in ethylene crackers. One of the consequences of this feedstock shift is that significantly less butadiene is made when ethane is cracked. The price of butadiene has increased from an average of \$0.60/lb prior to the discovery, to over \$1.60/lb today. This has increased pressure on making butadiene on purpose from other feedstocks.

1.5 Project constraints

Before and during World War II, this process was used in the United States and the Soviet Union. Since then it has not been used widely since it is less economical than the hydrocarbon extraction route, but it is still used in some parts of the world, such as China and India. The Ostromislensky process also has the benefit that it uses ethanol, a renewable resource, as its feedstock. A shift to this alternative production process would therefore reduce society's dependence on fossil fuels, a growing concern of our generation.

The United States and Brazil produce most of the world's ethanol by fermentation of local agricultural feedstock. The U.S. industry is almost entirely based on corn, while Brazil uses sugar cane. Process efficiencies in both countries have improved dramatically in recent years, with increasing ethanol production for use in transportation fuels.

2. Project Planning and Task Identification

2.1 Task identification

The task of our project was to successfully design a 1,3 butadiene production plant utilizing the Ostromislensky reaction that is capable of producing and purifying 200,000 tons of butadiene annually from local ethanol feedstock. All the while developing a profitable production process to convert ethanol to 1,3-butadiene with 98% purity.

2.2 Timelines

- Literature search (approx. 2- 3 weeks)
- Process selection (approx. 1 week)
- Flow sheet development (approx. 1.5 month)
- ASPEN HYSYS (approx. 3 weeks)
- Major Equipment Specifications (approx. 1 month)
- Economic Analysis (approx. 3 weeks)
- Reporting (approx. 2 months)

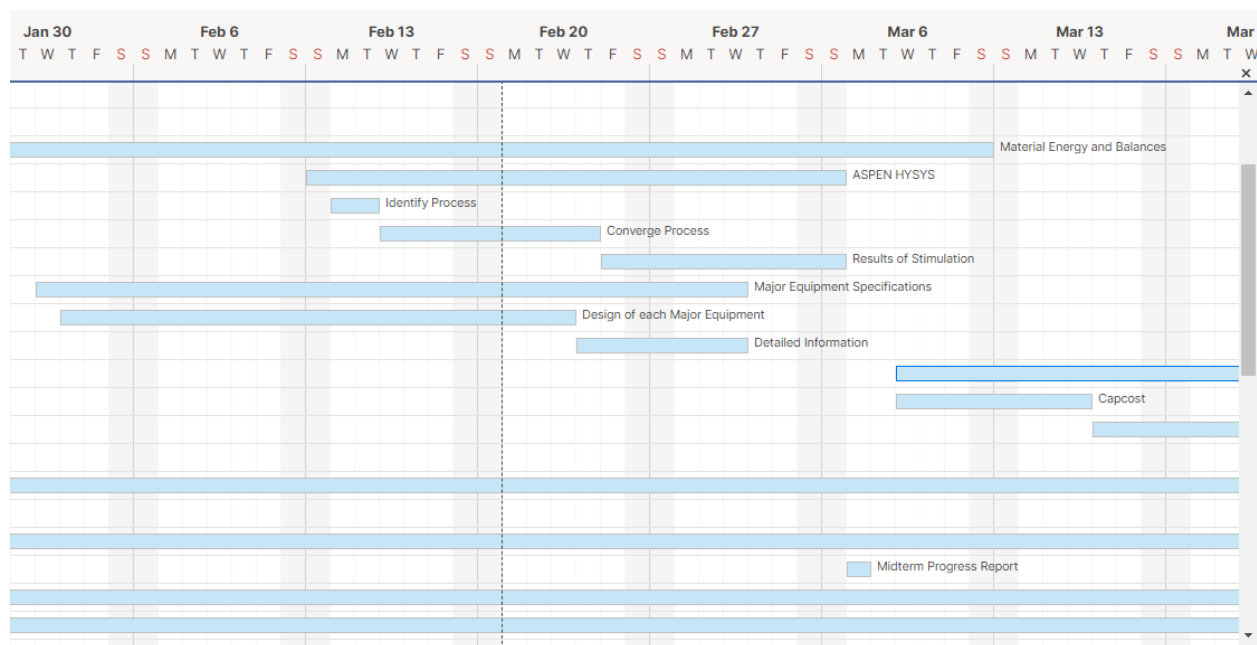
2.3 Gantt chart

2021-2022 GANTT CHART

1,3 Butadiene to Ethanol Plant Design

smartsheet

Tasks	Assigned To	Duration	Start Date	End Date
Literature Search		10 days	09/21/21	10/01/21
Project Selection		2 days	09/21/21	09/22/21
Initial Research		8 days	09/23/21	10/04/21
Process Selection		9 days	10/05/21	10/15/21
Process & Reaction		8 days	10/05/21	10/14/21
Flowsheet Development		33 days	10/15/21	11/30/21
Basic Information		7 days	10/15/21	10/23/21
Process Flow Diagram Draft		21 days	10/25/21	11/22/21
Material Energy and Balances		110 days	11/22/21	03/12/22
ASPEN HYSYS		21 days	02/13/22	03/06/22
Identify Process		2 days	02/14/22	02/15/22
Converge Process		8 days	02/16/22	02/24/22
Results of Stimulation		9 days	02/25/22	03/06/22
Major Equipment Specifications		26 days	02/02/22	03/02/22
Design of each Major Equipment		21 days	02/03/22	02/23/22
Detailed Information		7 days	02/24/22	03/02/22
Economic Analysis		22 days	03/09/22	03/31/22
Capcost		7 days	03/09/22	03/16/22
Cost Evaluation		7 days	03/17/22	03/24/22
Develop Cash Flow		7 days	03/25/22	03/31/22
Reporting		207 days	09/21/21	04/16/22
Selecting Process		2 days	09/21/21	09/22/21
Homework Assignments		198 days	09/21/21	04/09/22
Midterm Progress Report		TBD	TBD	03/07/22
End of the semester Report		86 days	01/20/22	04/16/22
End of semester Presentation		86 days	01/20/22	04/16/22



3. Literature review

3.1 overview of manufacturing of x,y,z & manufactured routes

1,3- butadiene is commonly produced as a byproduct when ethylene is produced through steam cracking of naphtha (paraffinic hydrocarbon) , also it can be produced through dehydrogenation / isomerization of n- butene through cracking of naphtha (Houdry process) ,another way to produce it from propylene currently 1,3 BD produced by steam cracking in olefin plants and the quantity of 1,3BD in this methods depends on the feedstocks used by cracker .or as in our report it can be maintained from 2 steps dehydrogenation using ethanol.

3.2 Physical and Chemical review

1,3- butadiene is a synthetic ,colorless gas or refrigerated liquid with mild aromatic or gasoline - like odor ,experimentally determined detection and recognition odor threshold

concentrations were 1.0 mg/m³(0.45 ppm) and 2.4 mg/m³ (1.1ppmv),stable ,extremely flammable it may form explosive with air ,incompatible with strong oxidizing, agent , phenol, chlorine , dioxide ,copper , copper alloy and crotonaldehyde it is insoluble in water but it is soluble in ethanol , ether acetone and benzene. It can easily ignite the properties of 1,3 butadiene.

1,3- butadiene properties:

Melting point	– 109 C
Boiling point	–4.5 C
Density	0.62 g/ml at 20 C
Vapor density	1.9 (15 C, VS air)
Vapor pressure	1863 mmHG (21 C)
Refractive index	1.4292
Flash point	–105 F , –76.1111 C
Storage temp.	0 –6 C
Solubility	Water : soluble 0.5 G/L at 20 C
form	Colorless gas
Explosive limit	12%

Odor threshold	0.23 ppm
Water solubility	735 mg/L at 25 C
Freezing point	-108.91 C
Molecular formula	C4H6
Formula weight	54.09
Exposure limit	TVL-TWA 10 ppm approximately 22mg/ m ³ (ACGIH) ,1000ppm (OSHAN & NIOSH) IDLH 20.000 ppm (NIOSH) , human carcinogen
Other name	Butadiene , alpha-gamma butadiene , bdivinyl , divinyl ,erythrene ,vinylethylene
Autoignition temp.	778 F , 414.444 C
Appearance	Colorless gas

3.3 Handling ,storage and safety

3.4 Handling

1,3- butadiene very toxic chemical , hazard require an expert advice on control to handle it in proper way we should follow some steps including label process container, provide each employee with hazard information and training to handle this product a person come in contact with this product should be trained in proper handling and safety per applicable federal , state and local laws and regulations , also using the personal protective equipment PPE like respiratory protection and person should not be assigned to tasks requiring the use of respirators unless it has been determined they are physically able to perform the work and are trained to use the equipments , beside wearing the chemical protective clothing CPC to prevent contact with chemicals that can injure or be absorbed through the skin . the skin that is in contact with butadiene may result in forstible. The level of protection selected should be based on the potential butadiene concentration and likelihood of contact; it could range from 0 CPC when

butadiene is handled in a closed system and there is no personal exposure , to fully encapsulating suits with supplied air respirators in certain spill situations.

The following table contains BD permeation test results for many of the most common cpc materials:

Table 4.2: Summary of Permeation Test Data for 1,3-Butadiene ⁵⁶⁷⁸			
Resistant Material	Breakthrough Time (hrs)	Permeation Rate ug/cm ² /min	Thickness
Butyl	>8.00	N/A ⁹	.07 cm
Natural Rubber	<0.02	637.27	.02 cm
Neoprene	0.78	1.80	.05 cm
PVC	<0.02	126.25	.02 cm
Tychem® BR	8.00	<.02	18 mils
Tychem® TK	8.00	<.07	25 mils
TRELLCHEM® EVO	>24.00	<.03	2 mils

Also the person who is in direct contact with BD should use appropriate eye and face protection. It is necessary to prevent contact with BD , exposure monitoring which is helping to detect if there is any exposure and the employee is responsible for ensuring the accuracy and precision of the method relevant to the unique condition .

3.5 Storage

1,3- butadiene must be stored outside or detached storage is preferred . the store is cool . dry well ventilated location isolated from oxidizing material . must be kept inhabited during storage . under pressure of thirty five F , should be kept away from heat , spark , hot surface ,open flames and other ignition

3.6 Safety

Will spilt the safety consideration into two parts , the first one is safety of equipment consideration The designing , so in this designing system the reaction is endothermic catalyst reaction which a hazard we might face is a thermal runaway reaction , the worst case scenario

should be considered and we suggest our producing system should has some specific equipment to consider what if or what is the worst case might happened which is another measure of risk to imagine the worst possible consequences . It is beneficial to avoid future or uncountable accidents or release of toxic substance in conclusion, our system needs relief valves on vessel line which open automatically at a certain pressure to avoid uncontrolled , catastrophic release of the contentment or destruction of the vessel , safeguards also one of our consideration which is used to relief the system under any unpredicted over heat generation release , also we might face some specific problem with our pump like cavitation which is formation of vapour bubble within the liquid at low pressure region that occurs in places where the liquid has been accelerated to high velocity and our team suggesting to have standby pumps and the routine check up of the equipment ...with distillation most likely the problem that we face is the large quantities of potential energy in the form of utility energy associated in the producing as know dealing with this kind of change it might cause huge massive risk and our system design as we discussed should attached with alarm system that indicate even the little or slightly change .

The other part of safety related to OSHA and NIOSH regulation on the 1,3-butadiene due the toxicity of it and the fact of this product being a carcinogen substance .

3.7.1 EPA & OSHA REGULATIONS

Under EPA's 1999 -guideline for carcinogen risk assessment (U.S EPA, 1999) 1,3 butadiene is characterized as carcinogenic to human by inhalation this characterization is supported by the total weight of evidence provided by the following ;sufficient evidence from epidemiologic studies of the the majority of U.S workers occupationally exposed to 1,3 – butadiene either to monomer or to the polymer by inhalation , showing increasing of lymphohematopoietic cancer and does a response relationship for leukemias in polymer worker , sufficient evidence in laboratory animal studies showing that the 1,3 butadiene cause tumors at multiple site in mice and rats by inhalation .

According to OSHA exposure to 1,3-butadiene can be cute low exposure , or cute high exposure and these document showing the OSHA regulation for BD

By [Standard Number](#) / 1910.1051 - 1,3-Butadiene.

▪ Part Number:	1910
▪ Part Number Title:	Occupational Safety and Health Standards
▪ Subpart:	1910 Subpart Z
▪ Subpart Title:	Toxic and Hazardous Substances
▪ Standard Number:	1910.1051
▪ Title:	1,3-Butadiene.
▪ Appendix:	A ; B ; C ; D ; E ; F
▪ GPO Source:	e-CFR

1910.1051(a)
Scope and application.

1910.1051(a)(1)
This section applies to all occupational exposures to 1,3-Butadiene (BD), Chemical Abstracts Service Registry No. 106-99-0, except as provided in paragraph (a)(2) of this section.

1910.1051(a)(2)(i)
Except for the recordkeeping provisions in paragraph (m)(1) of this section, this section does not apply to the processing, use, or handling of products containing BD or to other work operations and streams in which BD is present where objective data are reasonably relied upon that demonstrate the work operation or the product or the group of products or operations to which it belongs may not reasonably be foreseen to release BD in airborne concentrations at or above the action level or in excess of the STEL under the expected conditions of processing, use, or handling that will cause the greatest possible release or in any plausible accident.

1910.1051(a)(2)(ii)
This section also does not apply to work operations, products or streams where the only exposure to BD is from liquid mixtures containing 0.1% or less of BD by volume or the vapors released from such liquids, unless objective data become available that show that airborne concentrations generated by such mixtures can exceed the action level or STEL under reasonably predictable conditions of processing, use or handling that will cause the greatest possible release.

1910.1051(a)(2)(iii)
Except for labeling requirements and requirements for emergency response, this section does not apply to the storage, transportation, distribution or sale of BD or liquid mixtures in intact containers or in transportation pipelines sealed in such a manner as to fully contain BD vapors or liquid.

1910.1051(a)(3)
Where products or processes containing BD are exempted under paragraph (a)(2) of this section, the employer shall maintain records of the objective data supporting that exemption and the basis for the employer's reliance on the data, as provided in paragraph (m)(1) of this section.

1910.1051(b)
Definitions: For the purpose of this section, the following definitions shall apply:

Action level means a concentration of airborne BD of 0.5 ppm calculated as an eight (8)-hour time-weighted average.

Assistant Secretary means the Assistant Secretary of Labor for Occupational Safety and Health, U.S. Department of Labor, or designee.

Authorized person means any person specifically designated by the employer, whose duties require entrance into a regulated area, or a person entering such an area as a designated representative of employees to exercise the right to observe monitoring and measuring procedures under paragraph (d)(8) of this section, or a person designated under the Act or

regulations issued under the Act to enter a regulated area.

1,3-Butadiene means an organic compound with chemical formula $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$ that has a molecular weight of approximately 54.15 gm/mole.

Business day means any Monday through Friday, except those days designated as federal, state, local or company specific holidays.

Complete Blood Count (CBC) means laboratory tests performed on whole blood specimens and includes the following: White blood cell count (WBC), hematocrit (Hct), red blood count (RBC), hemoglobin (Hgb), differential count of white blood cells, red blood cell morphology, red blood cell indices, and platelet count.

Day means any part of a calendar day.

Director means the Director of the National Institute for Occupational Safety and Health (NIOSH), U.S. Department of Health and Human Services, or designee.

Emergency situation means any occurrence such as, but not limited to, equipment failure, rupture of containers, or failure of control equipment that may or does result in an uncontrolled significant release of BD.

Employee exposure means exposure of a worker to airborne concentrations of BD which would occur if the employee were not using respiratory protective equipment.

Objective data means monitoring data, or mathematical modelling or calculations based on composition, chemical and physical properties of a material, stream or product.

Permissible Exposure Limits, PELs means either the 8 hour Time Weighted Average (8-hr TWA) exposure or the Short-Term Exposure Limit (STEL).

Physician or other licensed health care professional is an individual whose legally permitted scope of practice (i.e., license, registration, or certification) allows him or her to independently provide or be delegated the responsibility to provide one or more of the specific health care services required by paragraph (k) of this section.

Regulated area means any area where airborne concentrations of BD exceed or can reasonably be expected to exceed the 8-hour time weighted average (8-hr TWA) exposure c ppm or the short-term exposure limit (STEL) of 5 ppm for 15 minutes.

1910.1051(d)
Exposure monitoring.

1910.1051(d)(1)
General.

1910.1051(d)(1)(i)
Determinations of employee exposure shall be made from breathing zone air samples that are representative of the 8-hour TWA and 15-minute short-term exposures of each employee.

1910.1051(d)(1)(ii)
Representative 8-hour TWA employee exposure shall be determined on the basis of one or more samples representing full-shift exposure for each shift and for each job classification in each work area.

1910.1051(d)(1)(iii)
Representative 15-minute short-term employee exposures shall be determined on the basis of one or more samples representing 15-minute exposures associated with operations that are most likely to produce exposures above the STEL for each shift and for each job classification in each work area.

1910.1051(d)(1)(iv)
Except for the initial monitoring required under paragraph (d)(2) of this section, where the employer can document that exposure levels are equivalent for similar operations on different work shifts, the employer need only determine representative employee exposure for that operation from the shift during which the highest exposure is expected.

1910.1051(d)(2)
Initial monitoring.

1910.1051(d)(2)(i)

Each employer who has a workplace or work operation covered by this section, shall perform initial monitoring to determine accurately the airborne concentrations of BD to which employees may be exposed, or shall rely on objective data pursuant to paragraph (a)(2)(i) of this section to fulfill this requirement. The initial monitoring required under this paragraph shall be completed within 60 days of the introduction of BD into the workplace.

1910.1051(d)(2)(ii)

Where the employer has monitored within two years prior to the effective date of this section and the monitoring satisfies all other requirements of this section, the employer may rely on such earlier monitoring results to satisfy the requirements of paragraph (d)(2)(i) of this section, provided that the conditions under which the initial monitoring was conducted have not changed in a manner that may result in new or additional exposures.

1910.1051(d)(3)

Periodic monitoring and its frequency.

1910.1051(d)(3)(i)

If the initial monitoring required by paragraph (d)(2) of this section reveals employee exposure to be at or above the action level but at or below both the 8-hour TWA limit and the STEL, the employer shall repeat the representative monitoring required by paragraph (d)(1) of this section every twelve months.

1910.1051(d)(3)(ii)

If the initial monitoring required by paragraph (d)(2) of this section reveals employee exposure to be above the 8-hour TWA limit, the employer shall repeat the representative monitoring required by paragraph (d)(1)(ii) of this section at least every three months until the employer has collected two samples per quarter (each at least 7 days apart) within a two-year period, after which such monitoring must occur at least every six months.

1910.1051(d)(3)(iii)

If the initial monitoring required by paragraph (d)(2) of this section reveals employee exposure to be above the STEL, the employer shall repeat the representative monitoring required by paragraph (d)(1)(iii) of this section at least every three months until the employer has collected two samples per quarter (each at least 7 days apart) within a two-year period, after which such monitoring must occur at least every six months.

1910.1051(d)(3)(iv)

The employer may alter the monitoring schedule from every six months to annually for any required representative monitoring for which two consecutive measurements taken at least 7 days apart indicate that employee exposure has decreased to or below the 8-hour TWA, but is at or above the action level.

1910.1051(d)(4)(i)

If the initial monitoring required by paragraph (d)(2) of this section reveals employee exposure to be below the action level and at or below the STEL, the employer may discontinue the monitoring for employees whose exposures are represented by the initial monitoring.

1910.1051(d)(4)(ii)

If the periodic monitoring required by paragraph (d)(3) of this section reveals that employee exposures, as indicated by at least two consecutive measurements taken at least 7 days apart, are below the action level and at or below the STEL, the employer may discontinue the monitoring for those employees who are represented by such monitoring.

1910.1051(d)(5)

Additional monitoring.

1910.1051(d)(5)(i)

The employer shall institute the exposure monitoring required under paragraph (d) of this section whenever there has been a change in the production, process, control equipment, personnel or work practices that may result in new or additional exposures to BD or when the employer has any reason to suspect that a change may result in new or additional exposures.

1910.1051(d)(5)(ii)

Whenever spills, leaks, ruptures or other breakdowns occur that may lead to employee exposure above the 8-hr TWA limit or above the STEL, the employer shall monitor [using leak source, such as direct reading instruments, area or personal monitoring], after the cleanup of the spill or repair of the leak, rupture or other breakdown, to ensure that exposures have returned to the level that existed prior to the incident.

1910.1051(d)(6)

Accuracy of monitoring. Monitoring shall be accurate, at a confidence level of 95 percent, to within plus or minus 25 percent for airborne concentrations of BD at or above the 1 ppm TWA limit and to within plus or minus 35 percent for airborne concentrations of BD at or above the action level of 0.5 ppm and below the 1 ppm TWA limit.

1910.1051(d)(7)

Employee notification of monitoring results.

1910.1051(d)(7)

Employee notification of monitoring results.

1910.1051(d)(7)(i)

The employer must, within 15 working days after the receipt of the results of any monitoring performed under this section, notify each affected employee of these results either individually in writing or by posting the results in an appropriate location that is accessible to employees.

1910.1051(d)(7)(ii)

The employer shall, within 15 business days after receipt of any monitoring performed under this section indicating the 8-hour TWA or STEL has been exceeded, provide the affected employees, in writing, with information on the corrective action being taken by the employer to reduce employee exposure to or below the 8-hour TWA or STEL and the schedule for completion of this action.

1910.1051(d)(8)

Observation of monitoring.

1910.1051(d)(8)(i)

Employee observation. The employer shall provide affected employees or their designated representatives an opportunity to observe any monitoring of employee exposure to BD conducted in accordance with paragraph (d) of this section.

1910.1051(d)(8)(ii)

Observation procedures. When observation of the monitoring of employee exposure to BD requires entry into an area where the use of protective clothing or equipment is required, the employer shall provide the observer at no cost with protective clothing and equipment, and shall ensure that the observer uses this equipment and complies with all other applicable safety and health procedures.

1910.1051(e)

Regulated areas.

1910.1051(e)(1)

The employer shall establish a regulated area wherever occupational exposures to airborne concentrations of BD exceed or can reasonably be expected to exceed the permissible exposure limits, either the 8-hr TWA or the STEL.

3.8 USAGE

1,3-butadiene is used widely in manufacturing synthetic rubber. It is intermediate in the manufacturing of adhesive synthetic and SBR is the primary material combined with natural rubber to make tires. The physical and chemical properties of these rubber polymers provide a high performance enhancing component to tires, such as rolling resistance, wear and traction. Also it is used in adhesives and sealants, as laboratory chemicals, automotive care products, lubricant and lubricant additives, paints and coating, plastic and rubber products.

4. Process Selection

4.1 Market Analysis and Trends

1,3-butadiene is a vital chemical compound used to make synthetic rubbers, polymers, resins, and a wide variety of other chemical intermediates. The major use of the compound 1-3 butadiene is in the manufacturing of tires.

1,3 butadiene is a monomer used to produce polymers for commercial and consumer applications. This compound is not used as a formulated ingredient. Many of the consumer goods and materials that are made of synthetic rubbers (elastomers), latexes, and plastics today contain the compound 1,3 butadiene. Elastomers made using 1,3-butadiene as a “building block” include styrene-butadiene rubber (SBR), polybutadiene rubber (PBR), polychloroprene (neoprene) and nitrile rubber (NR) (1,3-Butadiene).

Global consumption of butadiene is increasing annually by 4.1%. Since the demand for butadiene continues to exceed the domestic supply in most years, there tends to be a need for import rather than export. The demand in the global butadiene market is indicating reasonable growth – it is expected to grow at a rate of 3.9% annually over the next five to six years. However, the supply of butadiene grows at a rate of 2.0% annually. Factoring out developed countries, we can say that they are not considerable contributors to the demand growth due to the fact that the developed markets in developed countries have reached their saturation point. Brazil, Russia, India, and China are the developing BRIC countries that contribute to the growth in the market. This is principally due to the growing demand for SBR and polybutadiene rubber in these countries (Eldanel, 2010).

4.2 Reaction routes to producing product

Our plant has a production rate of approximately 200,000 tons per year, which would increase total production of butadiene globally by 2.0%. Plant expected to operate 90% of the year. Since the demand for 1,3 butadiene is constantly increasing, production levels are expected to increase as well as profit.

4.2.1 1,3 Butadiene industrial process and lab/patent routes have been reported to be used for producing 1,3 butadiene

PRODUCTION ROUTES	PROS	CONS
Extraction from C4 hydrocarbons	Cheap raw material	High operating cost Low selectivity Non sustainable Toxic
Dehydrogenation of n-butane	Cheap raw material	Low selectivity Less sustainable
Ethanol ✓	Cheap raw material Non toxic Biorenewable Environmental Friendly	Endothermic reaction requires high heating utilities
n-Butanol	Biorenewable	Endothermic reactions requires high heating utilities & Low selectivity

Table 4.2.1: Production Routes of 1,3 Butadiene

4.2.2 Reaction Route 1

The current method of producing 1,3 butadiene in the Western Europe, Japan, United States, and Western Europe is separating the compound from the stream mixture that is produced from the cracking of saturated hydrocarbons. A great amount of money is required to produce 1,3-butadiene. Ethane has become cheaper as a number of companies use it as a feedstock which becomes the main cause of lower production rate of butadiene. That is one of the main reasons why the price of butadiene increased from \$0.60/lb to \$1.01/lb.

4.2.3 Reaction Route 2

The production of 1,3 butadiene plays an important and useful role in the production of numerous different products since its demand is high. With the use of ethane resulting in a lowered production rate of 1,3 butadiene, other alternatives are essential. From here, it is necessary to find a profitable and sustainable way to mass produce 1,3 butadiene.

4.3 Process Screening Using Gross Profit Analysis

				Reaction 1 $\text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2$					(Dehydrogenation of Ethanol)							
				Reaction 2 $\text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_2\text{CHCHCH}_2 + 2 \text{H}_2\text{O}$					(Catalysis of Acetaldehyde)							
				Reaction 1						Reaction 2						
	Chemical Costs			kgmol	MW	kg	kg/kg	\$/ kg		kgmol	MW	kg	kg/kg	\$/ kg		
Ethanol	$\text{CH}_3\text{CH}_2\text{OH}$	\$0.338	lb	-1	46.07	-46.07	-1.0459	(\$0.35)		-1	46.07	-46.07	-0.8517	(\$0.29)		
Acetaldehy	CH_3CHO	\$0.46	lb	1	44.05	44.05	1	\$0.46		-1	44.05	-44.05	-0.8144	(\$0.37)		
Hydrogen	H_2	\$0	lb	1	2	2	0.0454	\$0.00		0	2	0	0	\$0.00		
1,3 Butad	H_2CHCHCH	\$1.01	lb	0	54.09	0	0	\$0.00		1	54.09	54.09	1	\$1.01		
Water	H_2O	\$0	lb	0	36.04	0	0	\$0.00		2	36.04	36.04	0.6663	\$0.00		
				Gross Profit Total=\$0.11/lb						Gross Profit Total= \$0.35/lb						

Table 4.3: Gross Profit Analysis of Acetaldehyde and 1,3 Butadiene

4.4 Process Comparison and Selection

There are two main methods for producing butadiene from ethanol: One step and Two-step. The two-step process named Ostromislensky was used during World War II. In that process, ethanol is first dehydrogenated to form acetaldehyde and then the ethanol-acetaldehyde mixture reacts further to form 1,3 butadiene and other byproducts. In Russia, a one step process was used. This process comprises the use of silicon-magnesium-chromium and silicon-magnesium tantalum catalyst. Ethanol reacts over the catalyst and the reactions are:

- $\text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2$ (1)
- $2 \text{CH}_3\text{CHO} \rightarrow \text{CH}_3(\text{CH})_3\text{O} + \text{H}_2\text{O}$ (2)
- $\text{CH}_3(\text{CH})_3\text{O} + \text{C}_2\text{H}_5\text{OH} \rightarrow \text{CH}_2\text{CHCHCH}_2 + \text{H}_2\text{O} + \text{CH}_3\text{CHO}$(3)
- $\text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_2\text{CHCHCH}_2 + 2 \text{H}_2\text{O}$(4)
- $2 \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_2\text{CHCHCH}_2 + \text{H}_2 + 2 \text{H}_2\text{O}$(5)

Comparing the two processes, they have similar intermediate reactions. The multi-step process seemed more appropriate since the intermediate reactions require different conditions to operate optimally. If the two-step reaction method is utilized, the first set of conditions can be set to maximize the dehydrogenation of ethanol and for the second set of conditions can be set to

maximize the reaction of acetaldehyde and ethanol. Furthermore, studies at the Mellon Institute in the 1950s showed that best yield obtained in the laboratory for the one-step process was 56%, whereas the best yield obtained for the two-step process was 64% (Corson, 1950). Based on information found by the group, we decided to use the two step- process. Studies showed that the two-step process provides a higher yield, and the byproducts were similar in both reactions. An assumption that the separation sections, and thus equipment costs, would remain the same. Furthermore, the dehydrogenation reaction of the two-step process utilizes relatively cheap catalysts. This helped to reduce any additional cost of two catalysts when being purchased. Using the two-step Ostromislensky process, helped to incorporate our feedstock, ethanol. Therefore, this reduced the society's dependence on fossil fuel. The two step Ostromislensky process was necessary to mass produce 1,3 butadiene because it is highly profitable. One key issue other manufacturers run into is the lower production rate of 1,3 butadiene. Issue was combated with the two-step process.

The first step of the process is an endothermic reaction because ethanol reacts over a heterogeneous catalyst to form acetaldehyde and hydrogen with a supply of heat. The Carbide and Carbon Chemicals Corporation specifies the selectivity of the reaction at 92%. The remaining 8% is associated with byproducts of the reaction which were not specified. The catalyst type and conversion were also not specified, therefore were viewed as design parameters that could be used to optimize the process (Burla, Fehnel, Louie, Terpeluk, 2012). Hydrogen was produced in a significant amount and requires a purification method for hydrogen.

The second step of the process will be endothermic as well because acetaldehyde and additional ethanol react over a packed bed of tantala-silica catalyst to form butadiene and water. The Carbide and Carbon Chemicals Corporation specifies a conversion of 44.5%, as well as a selectivity of 55%. Once again, it is assumed that the remaining 45% is associated with byproducts (Burla, Fehnel, Louie, Terpeluk, 2012). Diethyl ether, acetic acid, ethyl acetate, n-butanol, 1-butene, ethylene, and hexadiene are classified as main byproducts. As a significant amount of the reactants in the second step form unwanted byproducts, the process is required to separate 1,3-butadiene from the other byproducts. It will be cost efficient to recycle the remaining byproducts so the unreacted ethanol and acetaldehyde can react.

6. Process description

1,3 butadiene from ethanol plant design utilizes the two-step Ostromislensky process. The production capacity goal for the design is 200,000 metric tonnes per year. This capacity goal was reached by comparing competitor capacity goals and the demand for the 1,3-butadiene product. The process design's first step inputs ethanol into a catalytic dehydrogenation reactor to

convert ethanol into acetaldehyde and hydrogen. The process design's second step input introduces the acetaldehyde as intermediate to ethanol in a catalytic reactor to form butadiene. A hydrogen stream is created in this design which will be purified and sold when separated.

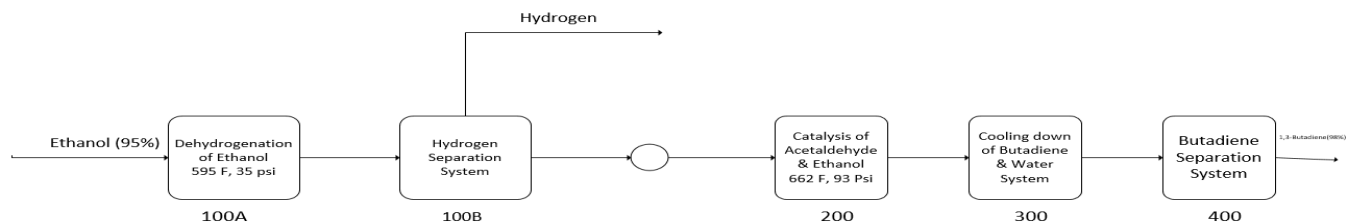


Figure 1: Block Flow Diagram of 1,3 butadiene process

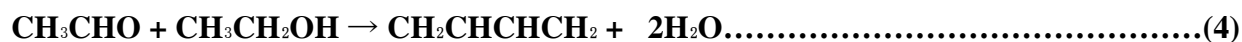
5.1 Process Chemistry

Step 1: Dehydrogenation of ethanol over a heterogeneous catalyst



In the first step of the process, ethanol reacts over a heterogeneous catalyst, copper-chromite, to form acetaldehyde and hydrogen with 92% selectivity on a shell-and-tube, packed bed reactor. The chosen catalyst in the first reaction, copper-chromite, has detailed kinetic parameters for dehydrogenation, allowing operating conditions to be optimized by simulation. Optimization for the first reactor was focused on obtaining an ethanol conversion of 50%. 50% was chosen because it minimized the amount of ethanol required for the entire process, without unnecessary waste. A significant amount of hydrogen is produced through the first reaction, and thus a process of separating and purifying the hydrogen is also required. The separated hydrogen is used as fuel for utility heat.

Step 2: Catalysis of Acetaldehyde



In the second step, the catalysis of Acetaldehyde is mixed with ethanol to form butadiene and water in a heterogeneous tantala-silica catalyst with 55% selectivity using the same type of

reactor as the first reaction. Finally, this last product goes through a distillation train to separate our final product 1,3 butadiene from the byproduct and recycle feeds, ethanol and acetaldehyde.

5.1.1 Reaction stoichiometry



..... (?)
..... (?)

5.1.2 Kinetics and rate equations

27

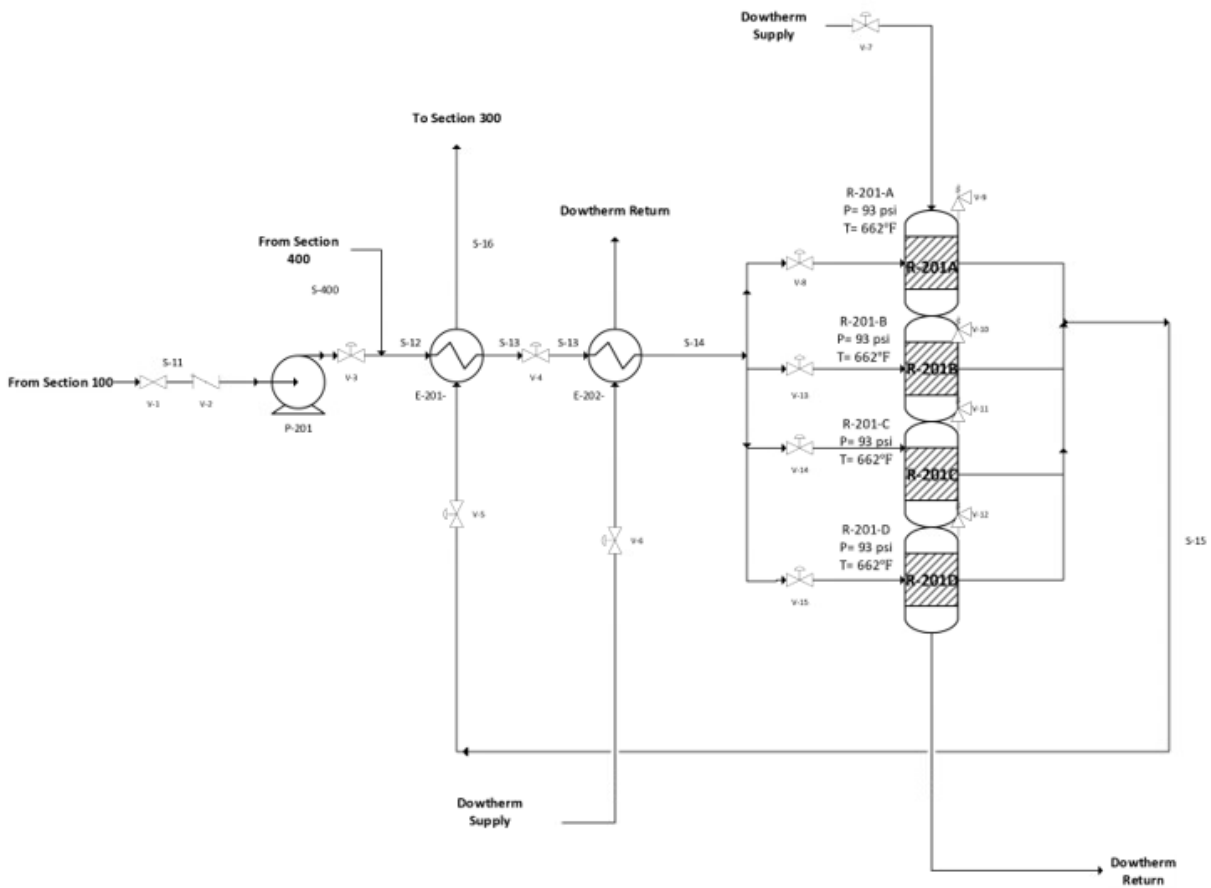


Figure 3: Section 200- Catalysis of Acetaldehyde & Ethanol

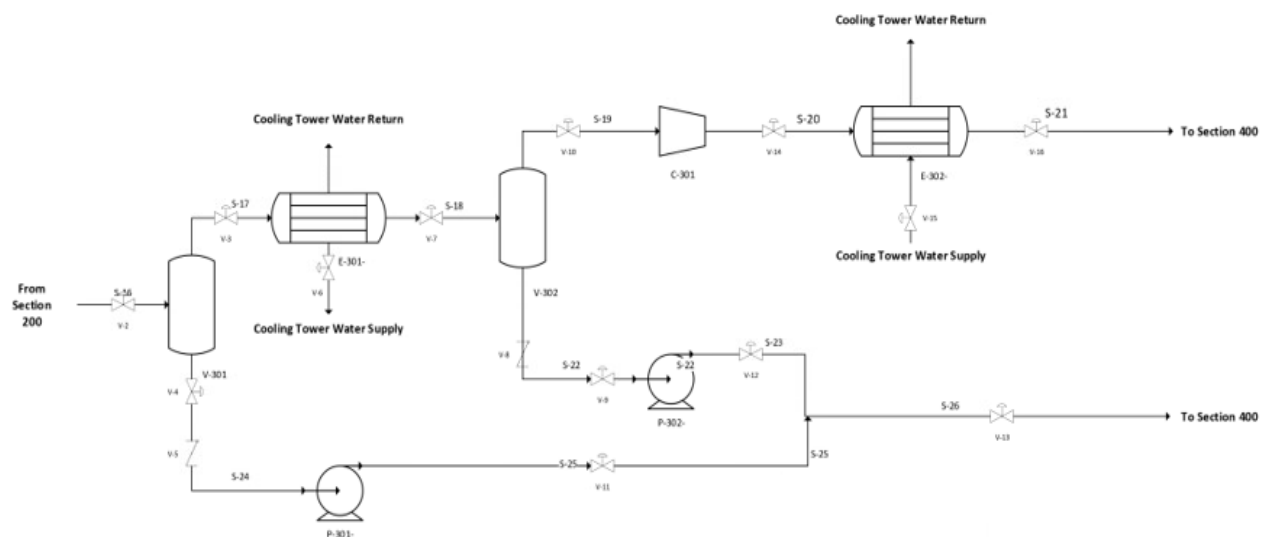


Figure 4: Section 300- Cooling Down of Butadiene & Cooling System

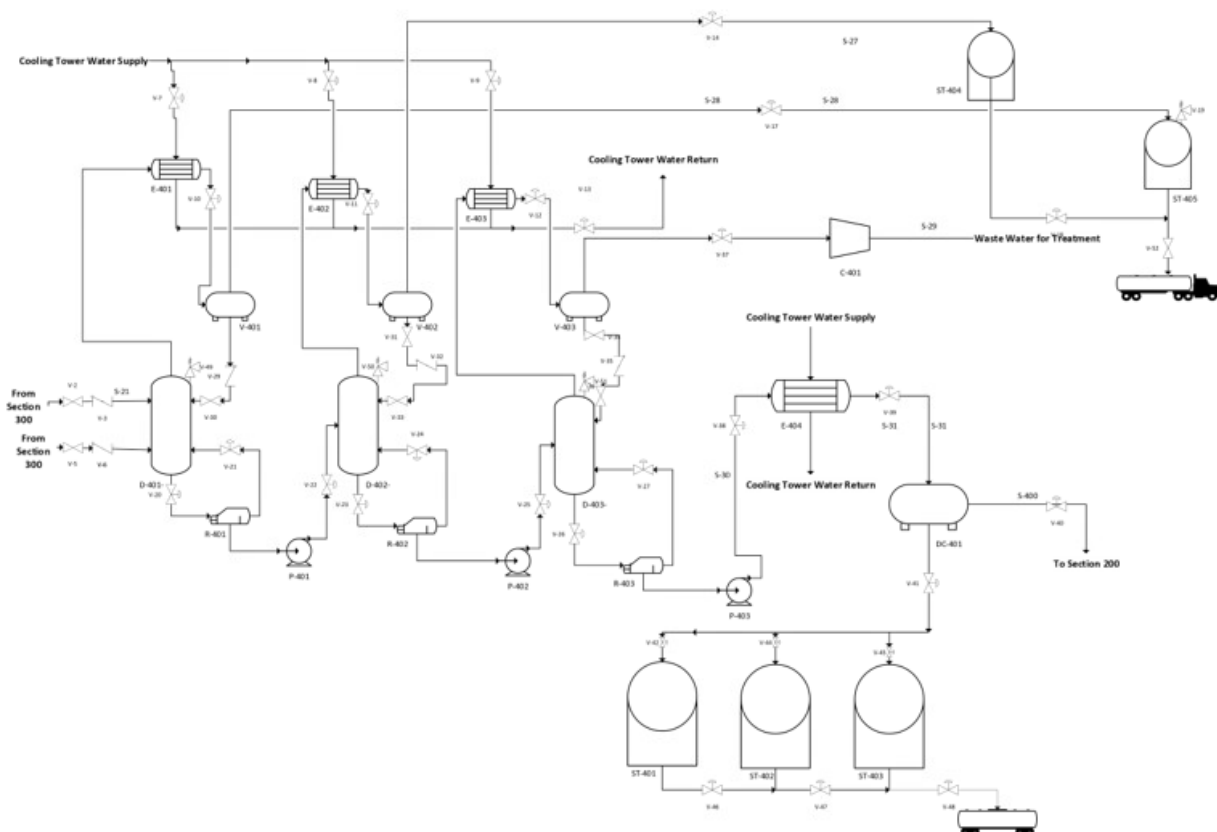


Figure 5: Section 400- Butadiene Separation System

5.2.1 Raw Material Preparation

The raw material preparation for this process consists of producing ethanol. Majority of the ethanol in the United States is produced from starch-based crops (corn) by dry- or wet-mill processing. Nearly 90% of ethanol plants are dry mills due to lower capital costs. Dry-milling is a process that grinds corn into flour and ferments it into ethanol with co-products of distillers grains and carbon dioxide. Wet-mill plants primarily produce corn sweeteners, along with ethanol and several other co-products (such as corn oil and starch). Wet mills separate starch,

protein, and fiber in corn prior to processing these components into products, such as ethanol (Ethanol Production and Distribution).

5.2.2 Reaction and reactor operation (Ostromislensky reaction)

- $\text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2$(1)
- $2 \text{CH}_3\text{CHO} \rightarrow \text{CH}_3(\text{CH})_3\text{O} + \text{H}_2\text{O}$(2)
- $\text{CH}_3(\text{CH})_3\text{O} + \text{C}_2\text{H}_5\text{OH} \rightarrow \text{CH}_2\text{CHCHCH}_2 + \text{H}_2\text{O} + \text{CH}_3\text{CHO}$(3)
- $\text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_2\text{CHCHCH}_2 + 2 \text{H}_2\text{O}$(4)
- $2 \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_2\text{CHCHCH}_2 + \text{H}_2 + 2 \text{H}_2\text{O}$(5)

Step 1: Heterogeneous catalyst in a fixed bed reactor (catalytic dehydrogenation

of ethanol to acetaldehyde and hydrogen)



Ethanol reacts over a heterogeneous catalyst to form acetaldehyde and hydrogen. The reaction is endothermic, therefore requiring a heating source (Dowtherm) to maintain operating conditions within the shell and tube-packed reactor. The Carbide and Carbon Chemicals Corporation specifies the selectivity of the reaction to be 92%. The remaining 8% is associated with byproducts of the reaction which were not specified. The catalyst type and conversion were also not specified and were therefore viewed as design parameters that could be used to optimize the process. A significant amount of hydrogen is produced in this reaction. A process of separating and purifying the hydrogen is essential.

Step 2: Heterogeneous catalyst in a fixed bed reactor (catalytic [tantala-promoted silica catalyst] acetaldehyde reacts with ethanol to form 1,3-butadiene and water)



In the second reaction, acetaldehyde and additional ethanol react over a packed bed of tantala-silica catalyst to form butadiene and water. Like the first reaction, the second reaction is endothermic and requires a heating source. The Carbide and Carbon Chemicals Corporation specifies a conversion of 44.5%, as well as a selectivity of 55%. Once again, it is assumed that the remaining 45% is associated with byproducts. The main byproducts include ethyl acetate, n-butanol, diethyl ether, acetic acid, 1-butene, ethylene, and hexadiene. Unlike the first reaction, a significant amount of the reactants in the second step form unwanted byproducts. Therefore, it is vital to have a process that separates the butadiene from the byproducts, as well as recycles back the unreacted ethanol- acetaldehyde.

5.2.3 Separations

Two separation units were used in our process. The separation units are responsible for separation products and recycle the unreacted reactants. The use of pressurized vessels was used to separate the various process streams into liquid and gas streams. Also, a pressure swing adsorber was used to purify out a hydrogen stream and to get rid of waste material. At the end of our process, there are a series of distillation columns which helps to reach our desired product purity.

5.2.4 Product to Storage

Our product, 1,3-butadiene, is stored in three separate storage spheres. The separate storage tanks serve as a checkpoint to verify each tank's composition/ specifications before it is sent out to clients. If any of the specifications are off, the tank is to be recycled back through the back end to undergo a further purification of the butadiene. After doing so, specifications should be ready to be sent out to clients.

6. Material and Energy Balances

6.1.1 Basis of calculations

The basis of calculation for our production of butadiene was determined by our market analysis of current and projected demand of butadiene compared to current and projected production. Our analysis determined that the target production capacity for our plant is 200,000 tons per year. This is our basis for calculation.

6.1.2 Material Balance around each unit

Name	Formula	MW (g/mol)	Section 100 Streams (mass fraction)									
			S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
Ethanol	C ₂ H ₆ O	46	.95	.95	.95	.95	.49	.49	.09	< .01	.11	.53
Acetaldehyde	C ₂ H ₄ O	44	-	-	-	-	.42	.42	.60	< .01	.83	.40
Hydrogen	H ₂	2	-	-	-	-	.02	.02	.26	.99	< .01	< .01
Methane	CH ₄	16	-	-	-	-	< .01	< .01	.01	< .01	.02	< .01
Water	H ₂ O	18	.05	.05	.05	.05	.05	.05	< .01	< .01	< .01	.05
Total (lb/hr)			155,000	155,000	155,000	155,000	155,000	155,000	11,700	3,000	8,700	143,300
Phase			Liquid	Liquid	Mixed	Vapor	Vapor	Mixed	Vapor	Vapor	Liquid	Liquid
Temperature (°F)			80	80	226	595	595	152	121	121	121	121
Pressure (psi)			15	50	42	35	30	22	155	155	155	155

Table 4: Section 100 Stream Information

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			Section 200 Streams (mass fraction)						
Name	Formula	MW (g/mol)	S11	S12	S13	S14	S15	S16	S400
Ethanol	C ₂ H ₆ O	46	.53	.67	.67	.67	.41	.41	.80
Acetaldehyde	C ₂ H ₄ O	44	.40	.23	.23	.23	.06	.06	.07
Diethyl-Ether	C ₄ H ₁₀ O	74	< .01	< .01	< .01	< .01	.04	.04	.01
Water	H ₂ O	18	.05	.07	.07	.07	.23	.23	.09
Total (lb/hr)			143,300	287,600	287,600	287,600	287,600	287,600	144,300
Phase			Liquid	Liquid	Vapor	Vapor	Vapor	Mixed	Liquid
Temperature (°F)			121	150	296	662	662	231	170
Pressure (psi)			155	108	100	93	73	66	108

Table 5: Section 200 Stream Information

			Section 300 Streams (mass fraction)										
Name	Formula	MW (g/mol)	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26
Ethanol	C ₂ H ₆ O	46	.41	.35	.35	.22	.22	.22	.57	.57	.48	.48	.51
Acetaldehyde	C ₂ H ₄ O	44	.06	.09	.09	.10	.10	.10	.06	.06	.03	.03	.04
Acetic Acid	C ₂ H ₄ O ₂	60	.01	< .01	< .01	< .01	< .01	< .01	< .01	< .01	.02	.02	.01
Diethyl-Ether	C ₄ H ₁₀ O	74	.04	.07	.07	.10	.10	.10	.02	.02	< .01	< .01	.01
Ethyl Acetate	C ₄ H ₈ O ₂	88	.01	.01	.01	.01	.01	.01	.01	.01	< .01	< .01	< .01
Water	H ₂ O	18	.23	.12	.12	.06	.06	.06	.21	.21	.38	.38	.32
Ethylene	C ₂ H ₄	28	< .01	.01	.01	.02	.02	.02	< .01	< .01	< .01	< .01	< .01
Hexadiene	C ₆ H ₁₀	80	< .01	< .01	< .01	< .01	< .01	< .01	.01	.01	.03	.03	.03
1,3-Butadiene	C ₄ H ₆	54	.20	.32	.32	.47	.47	.47	.09	.09	.03	.03	.05
Total (lb/hr)			287,600	163,400	163,400	99,900	99,900	99,900	63,500	63,500	124,200	124,200	187,700
Phase			Mixed	Vapor	Mixed	Vapor	Vapor	Mixed	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			231	231	200	200	282	200	200	200	231	231	221
Pressure (psi)			66	66	58	58	133	126	58	125	66	125	125

Table 6: Section 300 Stream Information

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Section 400 Streams (mass fraction)											
Name	Formula	MW (g/mol)	S-21	S-26	S-27	S-28	S-29	S-30	S-31	S-400	S-33
Ethanol	C ₂ H ₆ O	46	.22	.51	0	0	.03	.57	.57	.80	< .01
Acetaldehyde	C ₂ H ₄ O	44	.10	.04	< .01	0	.05	.05	.05	.07	< .01
Acetic Acid	C ₂ H ₄ O ₂	60	< .01	.01	0	0	.03	< .01	< .01	< .01	< .01
Diethyl-Ether	C ₄ H ₁₀ O	74	.10	.01	0	0	< .01	0	0	.02	< .01
Ethyl Acetate	C ₄ H ₈ O ₂	88	.01	< .01	0	0	.01	0	0	.02	< .01
Water	H ₂ O	18	.06	.32	.01	0	.83	.06	.06	.09	< .01
Ethylene	C ₂ H ₄	28	.02	< .01	.12	.79	.02	< .01	< .01	0	0
Hexadiene	C ₆ H ₁₀	80	< .01	.03	0	0	< .01	< .01	< .01	< .01	< .01
1,3-Butadiene	C ₄ H ₆	54	.47	.05	.82	.20	< .01	.28	.28	< .01	.99
Total (lb/hr)			99,900	187,700	800	2,340	84,460	200,000	200,000	144,300	55,700
Phase			Mixed	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)			200	221	108	17	110	215	170	170	110
Pressure (psi)			126	125	125	100	15	132	118	108	99

Table 7: Section 400 Stream Information

6.1.3 Overall material balance with process streams

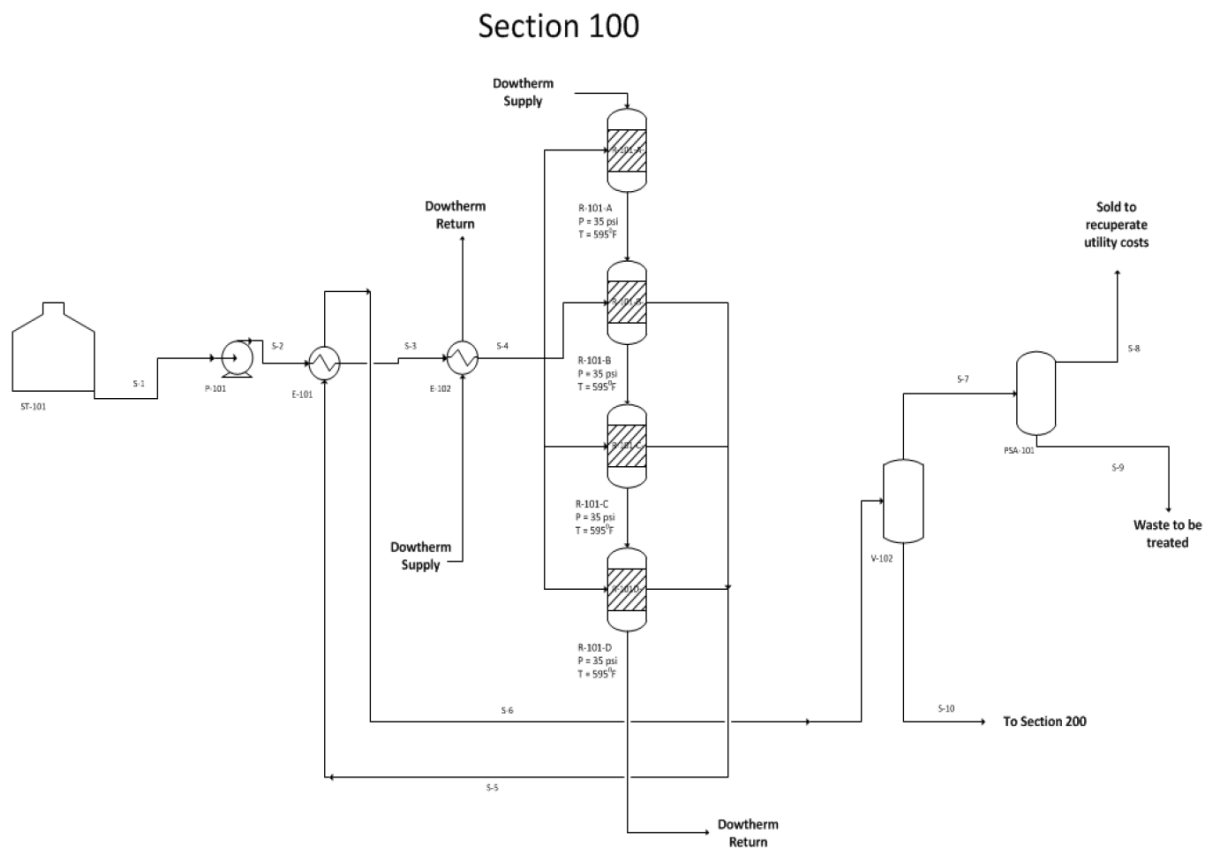


Figure 6: Overall Balance for Section 100

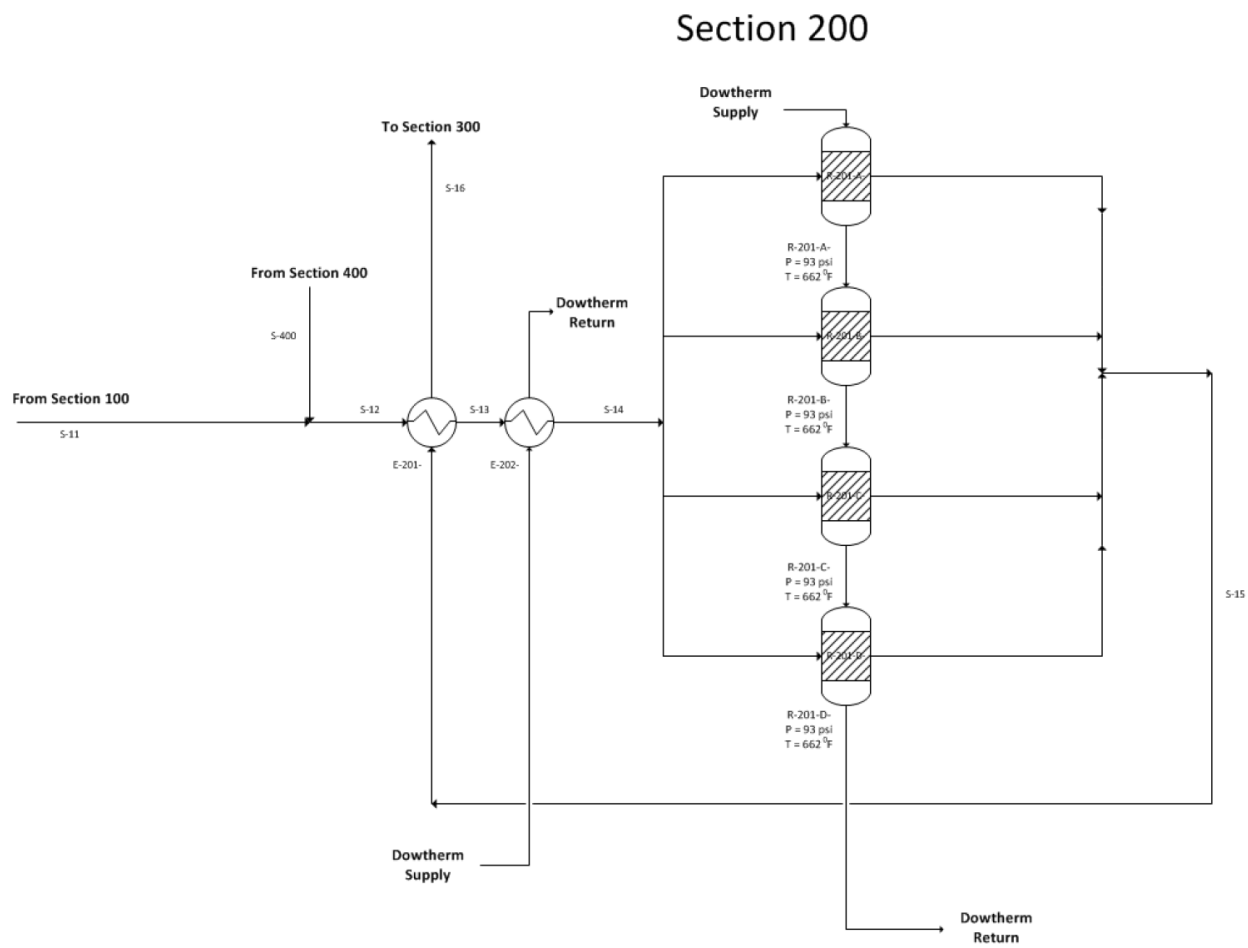


Figure 7: Overall Balance for Section 200

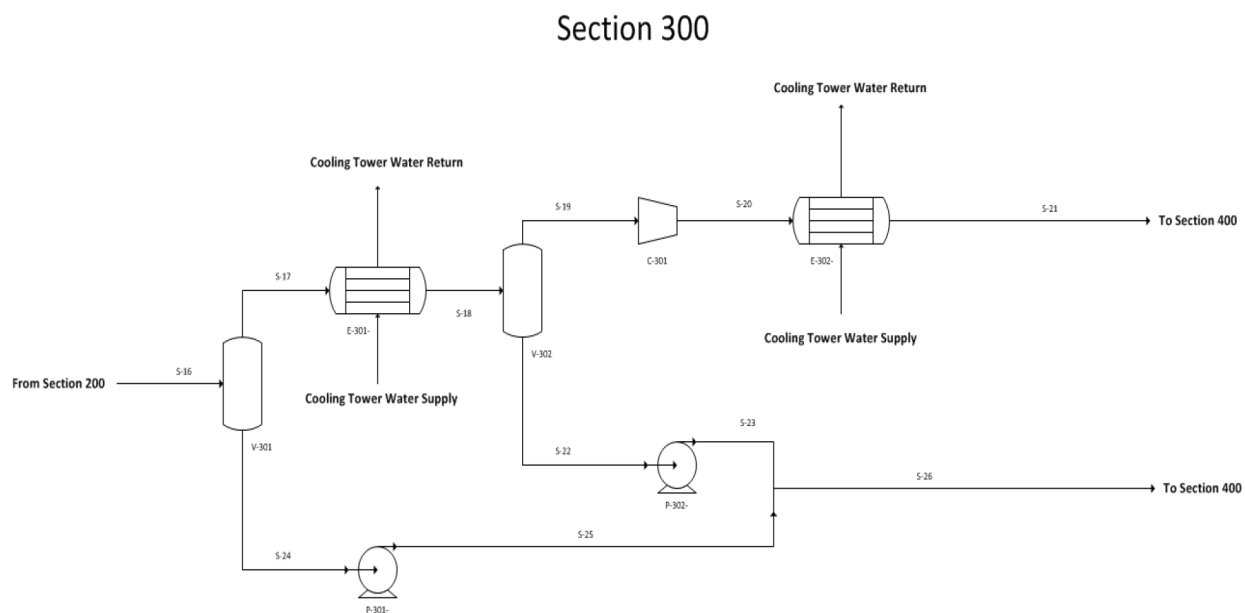


Figure 8: Overall Balance for Section 300

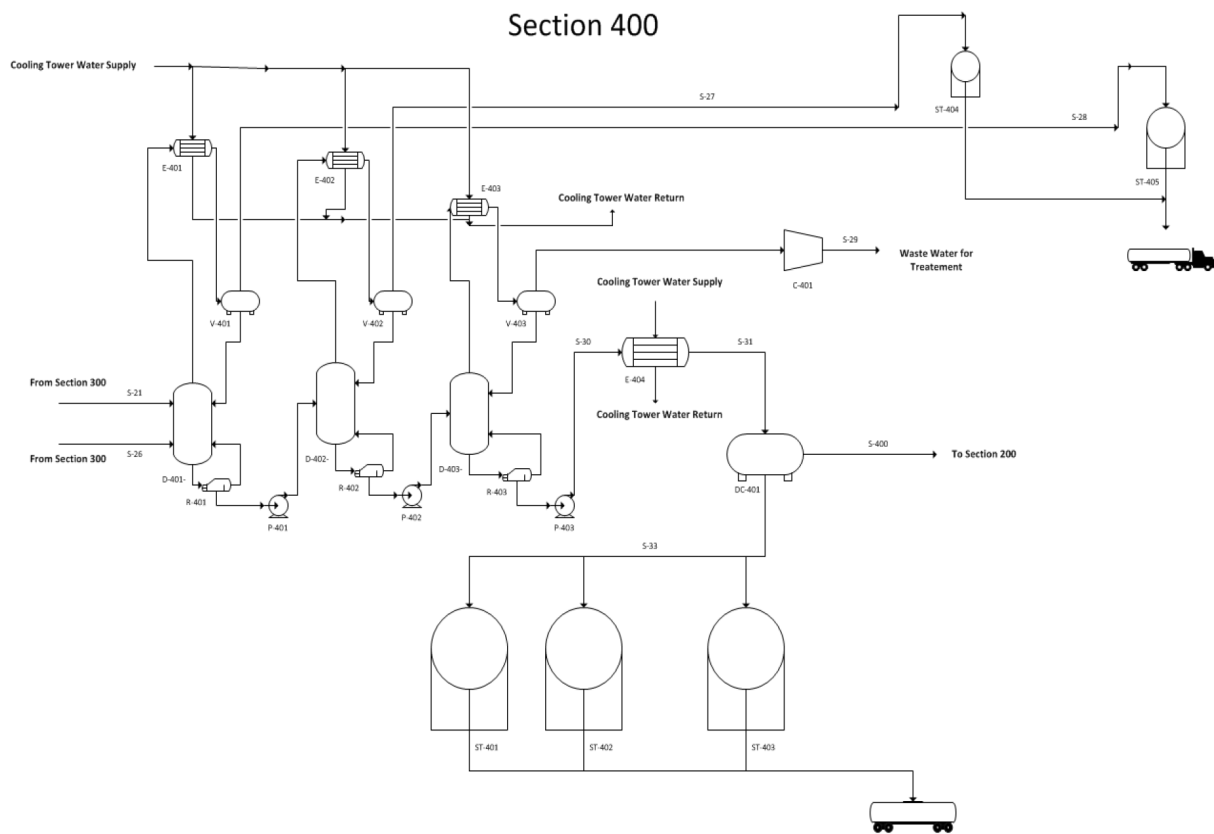


Figure 9: Overall Balance for Section 400

SECTION 100: DEHYDROGENATION OF ETHANOL

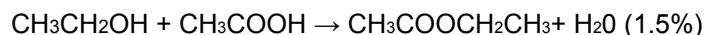
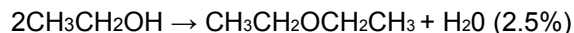
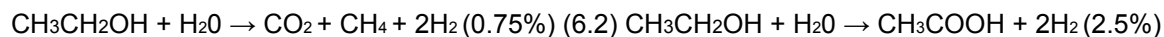
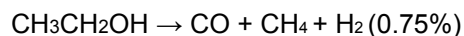
The first section contains one feed stream, a 95% ethanol and 5% water mixture (by mass), which enters the process from an API storage tank (ST-101, see p. 63) as a liquid at atmospheric pressure and a temperature of 80 °F. The storage tank has a holding time of seven days and uses nitrogen to maintain the ethanol in the liquid phase. The amount of feed required is 155,000 lb/hr, which is based on the conversion and selectivity of the two reactions and the desire to produce a total of 200,000 tonnes of butadiene per year. Furthermore, the Carbide and Carbon Chemicals Corporation has set the molar ratio of ethanol to acetaldehyde at 2.75:1 as the optimal inlet composition of the second reactor, which also dictates the feed flow rate.

The liquid feed stream is first pressurized to 50 psi (P-101, see p. 58) so that after pressure decreases in subsequent process equipment it will reach the first reactor at its optimum inlet pressure of 35 psi. The liquid stream is then sent to a heat exchanger (E-101, see p. 52) where it is heated to 226 °F and partially vaporized. E-101 uses the effluent of the first reactor as the heating fluid. The vapor/liquid stream then enters a pressurized vessel (F-101, see p. 56), where its two phases are split into separate streams. Both streams enter a single heat exchanger (E-102, see p. 53), where they are heated to the first reactor's optimum inlet temperature of 595 °F, at which temperature both streams are now in the vapor phase. E-102 is divided into two regions, an upper section for the inlet vapor stream and a lower section for the inlet liquid stream. The reason for separating the inlet streams is to ensure that both phases obtain equal contact with the heating fluid. E-102 utilizes vapor Dowtherm as its heating fluid.

The dehydrogenation reaction is carried out in a shell-and-tube, packed-bed reactor. The reactor is split between three shells in order to avoid purchasing costly large diameter units. Also, a fourth shell is purchased so that when one catalyst is being regenerated, continuous operation can be maintained. A heterogeneous copper-chromite catalyst is used to catalyze the endothermic reaction of ethanol to form acetaldehyde and hydrogen.



This reaction has a selectivity of 92%. The byproducts were not stated by the Carbide and Carbon Chemicals Corporation. Therefore the remaining 8% was estimated to include the following byproducts: carbon monoxide, carbon dioxide, methane, acetic acid, ethyl acetate, diethyl ether, and water. In order to model the reactor in ASPEN using RSTOIC, the following side reactions were assumed to occur (with respective selectivities):



The catalyst was chosen because detailed kinetic parameters were readily available for copper-chromite dehydrogenation, allowing operating conditions to be optimized by simulation. Optimization for the first reactor was focused on obtaining an ethanol conversion of 50%. 50% was chosen because it minimized the amount of ethanol required for the entire process, without unnecessary waste. If the conversion was higher than 50%, additional ethanol would have to be mixed with the inlet of the second reactor in order to maintain the required ethanol to acetaldehyde ratio of 2.75:1. Likewise, if the conversion was lower than 50%, the ethanol would have to be separated from the acetaldehyde leaving the first reactor in order to maintain the required ratio of the second reactor, and the amount of butadiene produced would be less than the desired 200,000 tonnes. This analysis was also dependent on how much ethanol and acetaldehyde could be recycled back to the second reactor. Therefore, a percentage recovery of ethanol and acetaldehyde after the second separation section (400) had to be determined before optimization of the first reactor could be executed.

After optimization, a final operating temperature of 595 °F and an inlet pressure of 35 psi were determined. The reactor is maintained at its isothermal temperature of 595°F using the Dowtherm heating system. Optimization also dictated the size and number of tubes required which affected the final cost of the reactor. The process of optimization and design for the reactors is detailed.

6.2 Energy Balances

Properties of Energy Balances

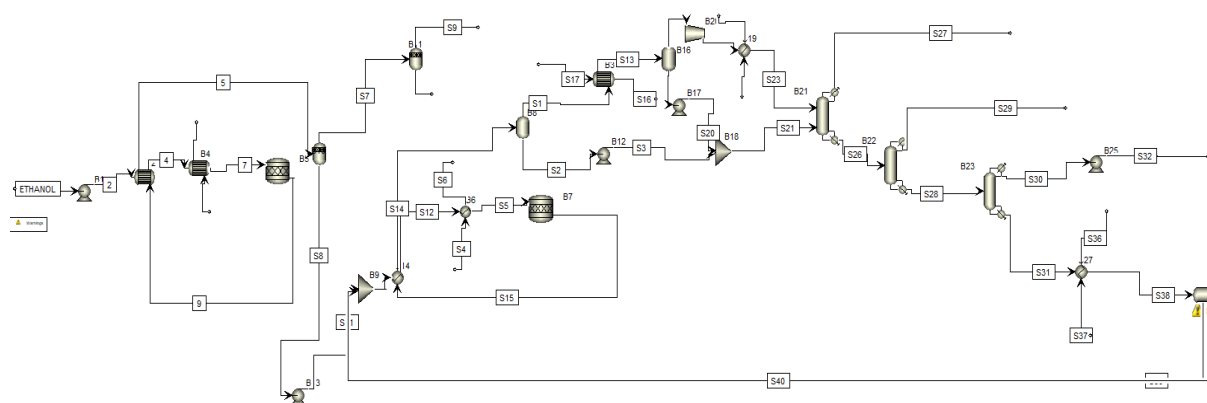
Multi-Stage Compressor	MSC-201	-60 MMBTU/hr to cool S9 from 152 °F to 107 °F	Cooling Water
Heat Exchanger	E-401	-30 MMBTU/hr to cool S28 from 231 °F to 200 °F	Cooling Water
Heat Exchanger	E-402	-20 MMBTU/hr to cool S31 from 281 °F to 200 °F	Cooling Water
Heat Exchanger	E-403	-78 MMBTU/hr to condense vapor at top of D-401 at 107 °F	Cooling Water
Heat Exchanger	E-408	-182 MMBTU/hr to condense vapor at top of D-403 at 193 °F	Cooling Water
Heat Exchanger	E-412	-83 MMBTU/hr to condense vapor at top of D-405 at 204 °F	Cooling Water
Heat Exchanger	E-414	-7 MMBTU/hr to cool S54 from 238°F to 110 °F	Cooling Water
Heat Exchanger	E-405	-3 MMBTU/hr to condense vapor at top of D2	Refrigeration
Heat Exchanger	E-410	-14 MMBTU/hr to condense vapor at top of D4	Refrigeration
Heat Exchanger	E-404	83 MMBTU/hr to boilup liquid in bottom of D-401	Steam
Heat Exchanger	E-406	5 MMBTU/hr to boilup liquid in bottom of D-402	Steam
Heat Exchanger	E-409	166 MMBTU/hr to boilup liquid in bottom of D-403	Steam
Heat Exchanger	E-411	13 MMBTU/hr to boilup liquid in bottom of D-404	Steam
Fired Heater	FH-501	100 MMBTU/hr to vaporize Dowtherm in S57 at 666 °F	Natural Gas
Fired Heater	FH-502	120 MMBTU/hr to vaporize Dowtherm in S61 at 625 °F	Natural Gas
Total Energy Requirement		110 MMBTU/hr	

Table 8: Energy Balance for process

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- R-101 Heat Duty: 46.3 MMBTU/hr to the reactor to keep the reactor isothermal.
- R-201 Heat Duty: 13.6 MMBTU/hr to the reactor to keep the reactor isothermal.

7. HYSYS/ASPEN Stimulation of Process



8. Chemical Engineering Design

8.1 Design of Major Equipment

DESIGN OF FIRST REACTOR

The values of all reactor specifications are stated below in the “Listing Equipment and Specifications”. We will only be focusing on the first reactor in this section. For the first reactor, the total mass flow rate was 150,000 lb/hr. The tube diameter was 0.125ft and the tubes was 20 feet long; the internal volume of one tube was 369 in^3 . The contact time (residence time) that occurred for the first reactor was approximately 5 seconds in one tube. This helped to get a superficial velocity of 4.0 ft/s, yielding 8,251 tubes. The volume of catalyst necessary is $1,764 \text{ ft}^3$. The shell dimensions of the first reactor are similar to the second reactor shell dimensions. Pitch required is $1.875 \text{ in}^2 \text{ pitch}$. Splitting the number of tubes between the four shells, 2,750 tubes are used in each shell which yields a shell diameter of 115 inches. The shell length is 24 feet long giving us 2 feet extra for the channeling. Using ASPEN, we calculated our heat duty of the first reactor to be 46.3 MMBTU/hr. The temperature of Dowtherm A fluid was held at a

constant 595 °F on the shell-side. We decided to operate the Dowtherm system for the first reactor at 606 °F, giving us a heat transfer coefficient of 67 BTU/°F-ft² -hr. Shell-side pressure was of 50 psi, which is close to the tube-side pressure of 32 psi needed for the thin-walled tube assumption.

REGENERATION OF CATALYSTS

Every 5 days, the catalyst must be regenerated by burning the carbon deposits coating the catalyst for six hours. The six hours of burning ensure the roughly 3% of the catalyst's weight being deposited doesn't reduce the efficiency of the catalyst. This time frame helps to keep the regeneration process within one working shift. "Therefore, one vessel will be offline for 30 hrs every five days, during which time it will undergo regeneration for eight hours- one hour for setup, six hours for regeneration and one hour for shutdown. Nitrogen was used in the inlet stream in order to absorb the heat of reaction, and maintain controllable reactor temperatures. The percent nitrogen in the flow was determined using ASPEN so as to set the temperature rise of the reactor at 400 °C, assuming the oxygen/nitrogen stream enters at 50 °C. Assuming an adiabatic temperature rise of 400 °C, it was found that the inlet stream should be 88% nitrogen. Thus, the nitrogen flow rate was determined to be 710,000 lb/five days for R-101." (Burla, Fehnel, Louie, Terpeluk)

Design of Pump

Pump is being used to supply the mixture of ethanol and acetaldehyde to reactor after being heated in E-201 and E-202.

In order to pump slurries, centrifugal pump can be used but with wider vanes and impeller used is open impeller in order to avoid wear from abrasion

8.2 Listing Equipment and Specification

EQUIPMENT	DESCRIPTION	Cp (cost of purchase, USD22)	EQUIPMENT PURCHASE COST
ST 101	Storage Tank	1,000,000	
P 101	Pump	24,400	
E 101	Heat Exchanger	135,000	
E 102	Heat Exchanger	667,000	
R 101	Reactor	183,000	
V 101	Pressurized Vessel	25,900	
PSA 101	Pressure swing adsorber	5,366,000	
E 201	Heat Exchanger	148,000	
E 202	Heat Exchanger	749,000	
R 201	Reactor	146,000	
	Sections 100 & 200 Cp Total (USD)	8,444,300	

EQUIPMENT	DESCRIPTION	Cp (Cost of purchase, USD22)
C 301	Centrifugal Compressor	1,030,000
E 301	Heat Exchanger	100,000
E 302	Heat Exchanger	79,000

P 301	Pump	9,825
P 302	Pump	8,123
V 301	Vertical Pressurized Vessel	25,400
V 302	Vertical Pressurized Vessel	17,900
	Section 300 Cp Total (USD)	1,270,248

EQUIPMENT	DESCRIPTION	Cp (cost of purchase, USD)
B 401	Kettle Reboiler	312,000
B 402	Kettle Reboiler	18,340
B 403	Kettle Reboiler	316,000
C 401	Centrifugal Compressor	1,349,300
D 401	Distillation Tower	612,000
D 402	Distillation Tower	447,000
D 403	Distillation Tower	583,000
DC 401	Decanter	31,500
E 401	Heat Exchanger	1,169,000
E 402	Heat Exchanger	86,500
E 403	Heat Exchanger	272,000
E 404	Heat Exchanger	36,500
P 401	Centrifugal Pump	25,000
P 402	Centrifugal Pump	22,000
P 403	Centrifugal Pump	10,000
ST 401	Special Pressurized Tank	593,500
ST 402	Special Pressurized Tank	232,000
ST 403	Vertical Pressurized Tank	593,500
ST 404	Vertical Pressurized Tank	593,500
	Section 400 Cp Total (USD)	5,953,340

Shell and Tube Packed Bed Reactor				
Identification:	Item: 4 parallel shells			
	Item No: R-101		Date: 03/10/2022	
	No. Required: 3		By:	JC
	Cost (\$):	183,000		
Function:	Dehydrogenation of ethanol into acetaldehyde and hydrogen gas			
Operation:	Continuous			
Materials Handled (lb/hr):	In	Out		
Ethanol	148,000	76,616		
Acetaldehyde	0	65,000		
Hydrogen	0	3,100		
Water	7,800	7,700		
Acetic Acid	0	535		
Ethyl Acetate	0	1,100		
Methane	0	200		
Carbon Dioxide	0	300		
Diethyl Ether	0	780		
Total Flow (lb/hr)	155,000	155,000		
Temperature (°F)	595	595		
Pressure (psi)	35	35		
Design Data:				
Type:	Floating Head, Shell and Tube			
Material:	Stainless Steel	Tube Length	20 ft	
Catalyst Type:	Copper- Chromite	Tube Diameter	0.125ft	
Catalyst Mass:	907,000 lbs	Number of Tubes	2750 per shell	
Number of Shells:	4	Residence Time:	5 s	
Heat Source	DowTherm	Utility (lb/hr):	407,000	

Shell and Tube Packed Bed Reactor				
Identification:	Item: 4 parallel shells			
	Item No: R-201		Date: 03/10/2022	
	No. Required: 3		By:	JC
	Cost (\$)	146,000		
Function:	To react acetaldehyde with excess ethanol to form 1,3- butadiene			
Operation:	Continuous			
Materials Handled (lb/hr):	In	Out		
Acetaldehyde	66,148	17,256		
1,3 butadiene	0	57,520		
Ethanol	192,692	117,916		
Water	20,132	66,148		
Total flow (lb/hr)	287,600	287,600		
Temperature (°F)	662	662		
Pressure (psi)	93	93		
Design Data:				
Type:	Fixed Head, Shell and tube	Tube Diameter:	0.12 ft	
Material:	Carbon Steel	Tube Length:	16 ft	
Catalyst Type:	2% tantala, 98% silica	Number of Tubes:	2,747	
Catalyst Mass:	230,000 lbs.	Shell Diameter:	115 in.	
Number of shells:	4	Residence Time:	5 s	

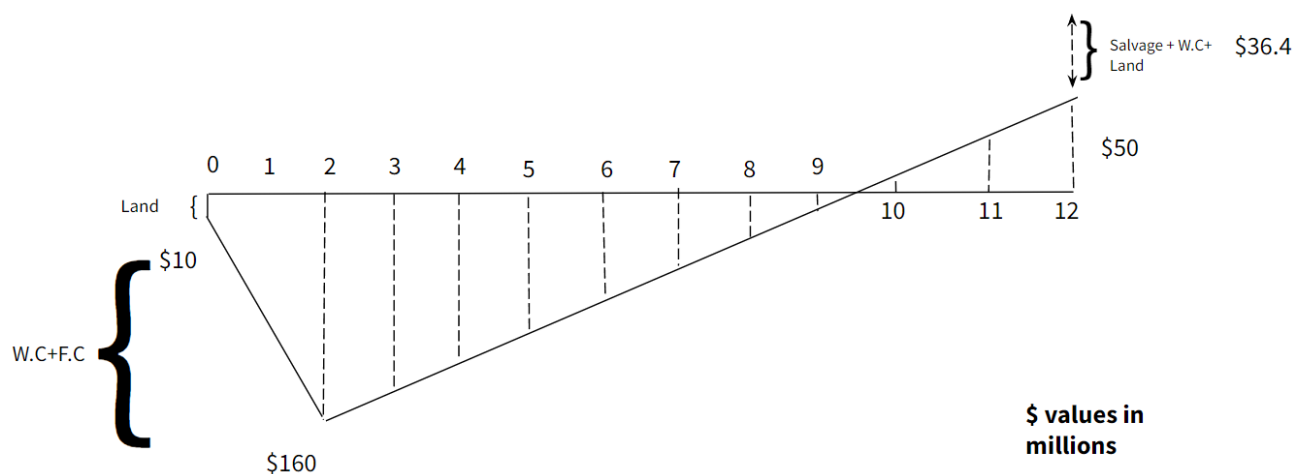
Heat Exchanger Data Sheet				Equipment No.: E-202	
				Descript. (Function): Heat Exchanger	
				Section No.: 200	
Operating Data					
Size (m)	6.1	Type	Pull Through	No. Of Units	1
Shells per Unit	1	Surface per Unit (m ²)			559.2
Performance of one Unit					
	SHELL SIDE			TUBE SIDE	
Fluid Circulating	Downstream A			Process Stream	
Total Fluid Entering (kg/hr)	772980.7			130457	
	IN	OUT		IN	OUT
Vapor	-	-		130457	130457
Liquid	772980.7	772980.7		-	-
Steam	-	-		-	-
Water	-	-		0	19050
Density (kg/m ³)	739.5	739.5		6.791	6.791
Molar Wt.	324.4			44.484	
Viscosity Liquid (Ns/m ²)	0.000155			0.0000126	
Latent Heat (kJ/kg)	-			-	
Specific Heat (kJ/kg-K)	2.537			2.0538	
Thermal Conductivity (W/m-K)	0.08466			0.0336	
Temperature (°C)	371.1	343.3		146.67	350
Operating Pressure (bar)	10	9		6.8	6.7
Velocity (m/s)	1.52	1.52		20.33	20.33
No. OF PASSES	1			2	
Pressure Drop (bar)	ALLOW	0.7	CALC 0.7	ALLOW	0.7
Heat Duty (kW)	15132.7			Mean Temperature Difference (K) 67.65	
Shell Side Heat Transfer Coefficient (W/m ² °C)	1331.7			Tube Side Heat Transfer Coefficient (W/m ² °C) 810.5	
Construction of Shell and Tube					
Tubes	989	Thickness (m)	0.002	Length (m)	6
Shell	1	I.D. (m)	1.382	Shell Cover	CS
Channel	CS	Channel Cover	CS	Floating Head Cover	CS
Tube Sheet Stationary	CS	Pull Through Floating Head			--
Baffles Cross	CS	Type	Single Segmental	Spacing % Cut	45%

HEAT EXCHANGER		
IDENTIFICATION: V-301		
FUNCTION: To change the phases of Ethanol and Butadiene from vapor to mixed		
OPERATION: Continuous		
Materials Handled: (lb/hr)	IN	OUT
1,3 Butadiene	52,288	52,288
Ethanol	57,190	57,190
Water	19,608	19,608
Total	163,400	163,400
DESIGN DATA:		
Type:	Shell-and-tube	
Material:	Carbon Steel	
Tube Diameter:	0.0625 ft	
Tube Length:	16 ft	
Number of tubes:	19	
Shell Diameter:	115 in	
Pressure In:	66 psi	
Pressure Out:	58 psi	
Area of Tube:	3.14 ft²	
T _{in} :	231°F	
T _{out} :	200°F	
UTILITIES: Cooling Water (1,937,584 btu/hr)		

HEAT EXCHANGER			
IDENTIFICATION: E-301			
FUNCTION: To cool part of reactor effluent, S17, to 200°F before it enters D-401			
OPERATION: Continuous			
Materials Handled:			
	(lb/hr)		
Acetaldehyde		14,110	
Acetic Acid		271	
Butadiene		52,952	
Diethyl Ether		11,769	
Ethanol		57,847	
Ethyl Acetate		1,972	
Ethylene		1,925	
Hexadiene		1,212	
Water		19,048	
Total		161,106	
DESIGN DATA:			
Type:	Shell-and-tube		
Material:	Carbon Steel		
Heat Transfer Area:	2,700 ft ²		
Length:	20 ft		
U:	100 BTU/ft ² -hr-°F		
Heat Duty:	30 MMBTU/hr		
Pressure Drop:	7 psi		
	<u>Hot Side</u>		<u>Cold Side</u>
T _{in} :	231°F		90°F
T _{out} :	200°F		120°F
UTILITIES: Cooling Water (1,000,000 lb/hr)			

Distillation Column				
Identification:	Item:	Distillation Column		
	Item No:	D-401	Date:	
	No. Required: 1		By:	JC
	Cost (\$)	612,000		
Function:	To separate the product, butadiene, along with ethylene, from the heavy products, including ethanol, acetaldehyde, and water.			
Operation:	Continuous			
	Feed	Distillate	Bottoms	
Materials Handled:				
	274,200	60,400	213,800	
Component Flow (lb/hr):				
Ethanol	118,500	0	118,500	
Acetaldehyde	18,000	700	17,300	
Diethyl-ether	13,000	1,500	13,000	
Water	66,000	1,500	64,500	
Ethylene	2,200	2,200	0	
1,3 butadiene	56,500	56,000	500	
Temperature (°F)	220	108	280	
Pressure (psi)	126	125	129	
Tower Design Data:				
Number of Stages	37	Tray Spacing (ft)	2	
Feed Stages	12	Inside Diameter (ft)	12	
Reflux Ratio	6	Height (ft)	86	
Column Material	Carbon Steel	Tray Material	Carbon Steel	
Tower Pressure (psi)	125	Tray Type	Sieve	
Operating Temperature (°F)	Within 108-280			
Associated Components				
	Parameter	Value		
Tower				
	Equipment Type	Vertical Vessel		
	Weight (lbs.)	165,000		
	Thickness (in)	2.5		
	Bare Module Cost			
Condenser				
	Equipment Type	Fixed Head Heat Exchanger		
	Heat Duty	.78 MMBTU/ hr		
	Shell Material	Carbon Steel		

9. Economic Evaluation



Net Present Value (NPV)	(\$30,964,090.78)
Investor's Rate of return	3%
Payback Period (yrs)	7.619
Fixed Capital Investment (FC)	\$136,000,000
Working Capital (WC)	\$24,000,000
Land	\$10,000,000

To do an overall profitability analysis of the proposed manufacturing design of 1,3-butadiene, a cost analysis was done for the overall cost of the facility. This analysis consisted first of determining the cost of the land for the site. A professional real estate group in our facility's state of Texas, it was determined that the land required for the site would cost \$10,000,000.

10. Safety and HAZOP Analysis

HAZOP Study

The objectives of the study are:

1. To identify major problems involved in separation of methanol from water.
2. To study safety measures and possible precautions in practice.
3. To identify and determine major hazards potential in the process equipment.
4. Give suggestions to minimize risk by reducing hazard and probability.

- ☐ 1,3 Butadiene is extremely flammable.
- ☐ May cause an explosive mixture with air.
- ☐ May cause frostbite.
- ☐ Contains gas under pressure; may explode if heated.
- ☐ Inhalation may cause cancer and genetic defects.
- ☐ Hydrogen has a wide flammability range, and can form an explosive mixture with air.
- ☐ Hydrogen can be explosive at concentrations of 18.3%-59%.
- ☐ Gaseous hydrogen cannot be detected by the human senses, and its flame is also invisible.
- ☐ Hydrogen diffuses through materials not normally considered porous.
- ☐ Handling liquid hydrogen can bring evaporation problems that require adopting certain measures.
- ☐ Leaks have to be controlled.
- ☐ Due to its small size, hydrogen can cause embrittlement of high strength steels, titanium and aluminum alloys, with cracking and catastrophic failure of the metals.
- ☐ Hydrogen requires only a small amount of energy for ignition (0.02 mJ).

Process parameter	Deviation	Possible consequences	Possible causes	Action required/ Safeguards
Pressure	More	- High/rising velocity of reactant - Overpressure of the process - High/rising temperature	- Valve failure - Overheating of the column/separator	- Installation of High pressure/ High temperature alarm - Installation of safety valve
	Less	- Less reaction - Less favorable product	- Leakage in the process - Compressor failure	- Insertion of safety valve - Installation of low pressure alarm
Temperature	More	- Uncontrolled reaction - Mechanical failure - May cause explosion	- Pressure/temperature instrument failure - Too much heat supplied from the heat source - Fan failure	Installation of temperature/pressure sensor
	Less	Less pressure, less favorable product.	Too little heat supplied from the heat source	Installation of temperature/pressure sensor
Ignition	-	- Fire, sparks - Runaway reactions - Explosion	- Presence of oxidizing substance - Temperature rise	- Insulation of piping and equipment - Temperature sensor

HAZOP study of Heat Exchanger (E-202)

Heat exchanger E-202 is used to increase the reactor feed temperature to a desired level so that reaction may be performed in the reactor. Downtherm A is being used to increase the temperature. Line from (with conditions as 662 °F, 93 psia and 287600 lb/h) heat exchanger E-202 to the reactor inlet is selected for HAZOP.

Keyword	Guide word	Deviation	Causes	Consequence	Action
Flow	No	No flow of Downtherm A	Failure of inlet Downtherm A valve to open	Desired temperature of reactor inlet feed is not achieved	Install temperature indicator and alarm to indicate the malfunction
	More	More flow of Downtherm A	Failure of inlet Downtherm A valve to close	Temperature of reactor inlet feed is exceeds beyond a certain desired point	Install temperature controller and high temperature alarm
	Less	Less flow of Downtherm A	Pipe leak	Desired temperature of reactor inlet feed is not achieved	Install temperature controller and low temperature alarm
Pressure	High	Out let pressure of reactor inlet feed is high	Increased pressure from pump	High pressure can affect the efficiency of the reactor. Moreover, it can	Control the pressure of feed. Install high pressure alarm. Install rupture disk on the pipeline to save the

				result in failure of pipe or vessel.	equipment due to increased pressure.
Temperature	High	High temperature of reactor inlet feed	Increased inlet Downtherm A flow	Temperature of reactor inlet feed is exceeds beyond a certain desired point	Install temperature controller and high temperature alarm
	Low	low temperature of reactor inlet feed	Decreased inlet Downtherm A flow	Desired temperature of reactor inlet feed is not achieved	Install temperature controller and low temperature alarm

Piping and Instrumentation

Different instruments and control loops are being implemented on the section 200 to ensure the safe, smooth and reliable operation, good quality of product, etc.

Temperature Controller

Temperature of feed inlet to the reactors is controlled by manipulating the flowrate of Downherm A to the heat exchanger (E-202). Temperature of reactor inlet feed is measured and transmitted to the controller where set point is given. Controller calculates the error and changes the valve opening accordingly to control the temperature. Similarly, temperature of reactor outlet is controlled by manipulating the flowrate of Dowtherm A to the reactors.

Connection of control valve

Every control valve has a connection whether it is air to open or air to close

In section 200 we have air to open in case of emergency will be close and action will be based on safety if we need to get extra safety to our equipments if it is cooling will be air to close in case of emergency we need to put flow rate to cool our equipments

In section 200 we have heating flow rate so will be air to open in case of emergency will be air to close and no downtherm will be provide

Pressure safety valve

In case of emergency or increasing of pressure buoyed the designing pressure , pressure safety valve will pup up . Stream will be out to safe location and our equipments will be safe

Shuttle valve

To avoid any case of emergency we can shut in order to avoid the usage of the section , usually will be open during the normal process that doesn't apply any emergency cases .

Isolation valve

To isolated in case of maintenance so it can isolate the required section

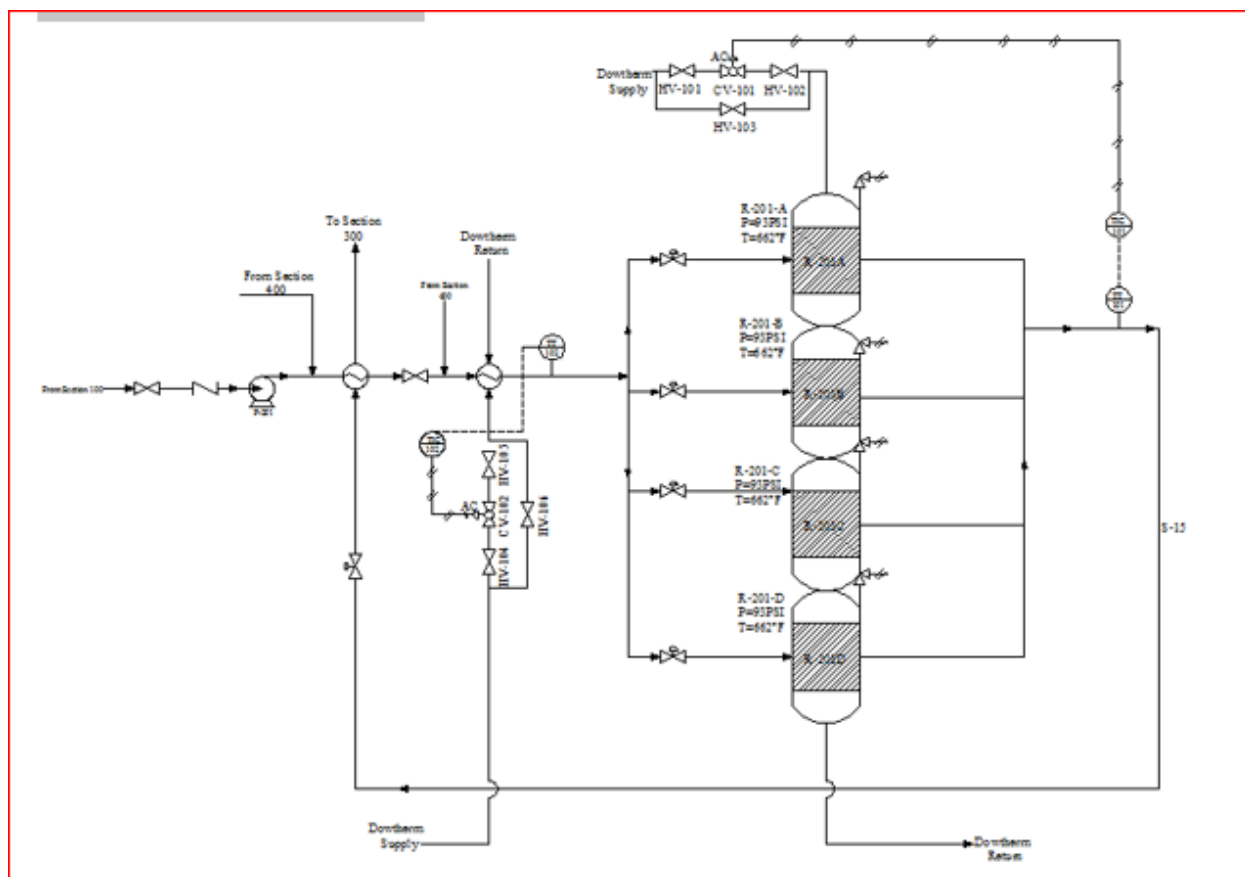


Figure : Piping and instrumentation diagram on section 200

Discussions:

In summary, this project scope provides a first look into the design of a two-step production of 1, 3-butadiene. This route strategically uses a feedstock of ethanol to best provide an economically feasible polymer grade product. The location of the plant also helps to drive down the overall production cost of butadiene. Decatur provides local access to our feedstock which ensures the lowest possible transportation costs of our feedstock. Based on our financial analysis, this design will generate a great return on investment over time.

Going forward, considerations which need to be analyzed are as follows:

- Continue to monitor the 1,3-butadiene market
- Reevaluate profitability after ten years of operation
- Continue to update standard operating procedures with a key focus on safety
- Instruct plan for saving energy on plant
- Find a way to reduce the overall investment

Conclusion and Recommendations:

After thorough investigation of the two-step catalytic process of converting ethanol to 1,3 butadiene, we have concluded that the process would be a promising venture. Although the project requires a significant initial total capital investment of \$136 million, the potential for large profit combined with a growing demand for butadiene allows the project to look more profitable in the coming years. The design achieves the 200,00 tonne target production level of 98% purity from butadiene per year and the results of ROI of 3% and a NPV of \$31 million. With butadiene's importance in the global rubber industry and reductions in production rates of butadiene from hydrocarbon extraction, investing in a butadiene plant shows a very promising business venture. The overall economics and analysis show that this project will be profitable following recent market trends. Ethanol plays a significant proportion of the total variable cost and its market prices play an important role as well in our design. With ethanol production increasing, which results in an increasing availability and relatively stable prices, butadiene is increasing as well. These two market trends are boosting the profitability of this plant. Based on our investigation of the plant design, we have devised key recommendations as to what should be studied further if our design is pursued. First, a large amount of acetaldehyde is lost in this process. Continuous look into separation technologies should be investigated to help reduce this issue. If more acetaldehyde is recovered, then ethanol would have to be initially dehydrogenated. Another suggestion would be increasing the capacity of the reactor so we could recycle back more of the effluent streams. Allowing this to do so would include an economic analysis to determine if the increased recovery of acetaldehyde is worth making modifications. Keeping these in mind, construction of a plant with 200,000 tonnes per year of butadiene is strongly recommended. Major factors of consideration in this decision are the 3% rate of return with the encouraging market trends of both butadiene and ethanol.

Appendix:

Relevant Calculations for R-101 & R-201

- Volume of Ethanol: $V_{\text{ethanol}} = \frac{n_{\text{ethanol}} \cdot MW}{\rho_{\text{ethanol}}}$
- Tube Bundle Internal Volume Calculation: $V = \pi \cdot (\text{tube inner radius})^2 \cdot L_{\text{tube}}$
- Number of tubes: $N_t = \frac{\text{total volumetric flowrate}}{\text{volumetric flowrate}_{\text{one tube}}}$, with
 - $\text{Volumetric flowrate}_{\text{one tube}} = \frac{\text{tube volume}}{\text{contact time}}$
- Superficial velocity through a tube: $V_{\text{one tube}} = \frac{\text{Volumetric flowrate}_{\text{one tube}}}{\text{cross sectional area of one tube}}$
- Volume of catalyst: $V_{\text{catalyst}} = N_t \cdot \text{Volumetric flowrate}_{\text{one tube}}$
- Tube side pressure drop:

$$\Delta P = \frac{150 \cdot \mu_{\text{fluid}} \cdot (1-\epsilon)^2 \cdot L_{\text{tube}}}{0.5^3 \cdot D_p \cdot z^3} \cdot V_{\text{superficial}} + \frac{1.75 \cdot \mu_{\text{fluid}} \cdot (1-\epsilon)^2 \cdot L_{\text{tube}}}{0.5^3 \cdot D_p \cdot z^3} \cdot (V_{\text{superficial}})^2$$
- Shell Diameter: $D_S = \sqrt{\left(\frac{N_t}{3} \cdot (\text{square pitch})^2 \cdot \frac{4}{\pi}\right)} + 2 \cdot \text{tube outer diameter} + 1$
- Heat transfer coefficient: $U = \frac{Q}{A \cdot \Delta T}$

Unit Descriptions:

COMPRESSORS

C-301 is a carbon steel, centrifugal compressor. It is used to pressurize stream S19, with a flowrate of 100,000 lb/hr from 58 psi to 133 psi. The compressor has a capacity of 250,000 ft³/hr and an efficiency of 72%. The estimated purchase cost is \$1,030,000.00.

DISTILLATION COLUMNS

DECANTERS

HEAT EXCHANGERS

E-301 is a shell-and-tube heat exchanger fabricated from carbon steel. It uses cooling water with a flow rate of 1,000,000 lb/hr to further cool the second reactor's effluent stream S17 which had a flow rate of 160,000lb/hr. This cools S17 from 231°F to 200°F and condenses 45% of the stream. The cooling water is heated from 90°F to 120°F. This process transfers 30 MMBTU/hr. The estimated purchase cost of E-301 is \$100,000.00.

E-302 is a shell-and-tube heat exchanger fabricated from carbon steel. It uses cooling water with a flowrate of 670,000 lb/hr to further cool the second reactor's effluent now leaving the compressor. Stream S20 which has a flow rate of 100,000 lb/hr. This cools S20 from 282°F to 200°F and condenses 65% of the stream. The cooling water is heated from 90°F to 120°F. Stream S21 is now at the optimal inlet temperature for the first distillation column, D-401. This process transfers 20 MMBTU/hr of heat. The estimated cost purchase is \$79,000.00.

PRESSURIZED VESSELS

V-301 is a carbon steel, vertical pressurized vessel. It is used to separate the vapor and liquid phases from stream S16 which has a flow rate of 290,000 lb/hr. The vapor product S17 has a flow rate of 160,000 lb/hr and the liquid product S24 has a flow rate of 130,000 lb/hr. It has a diameter of 9.5ft. It operates at 66 psi and 231°F. The estimated cost purchase is \$25,400.00.

V-302 is a carbon steel, vertical pressurized vessel. It is used to separate the vapor and liquid phases from S18 which has a flow rate of 160,000 lb/hr. The vapor product stream S19 has a flow rate 100,000lb/hr and the liquid product stream S22 has a flow rate of 60,000 lb/hr. It has a diameter of 9.5ft. It operates at 58 psi and 200°F. The estimated purchase cost is \$17,900.00.

PUMPS

P-301 is a carbon steel, centrifugal pump. It is used to pressurize stream S24 with a flowrate of 63,000 lb/hr. The pressure of S24 increased from 58 psi to 125 psi. The pump capacity is 1,400 ft³/hr and efficiency of 60% The estimated purchase cost is \$9,825.00.

P-302 is a carbon steel, centrifugal pump. It is used to pressurize stream S22 with a flowrate of 120,00 lb/hr. The pressure increased from 66 psi to 125 psi. The pump has a capacity of 2,600 ft³/hr and efficiency of 67%. The estimated purchase cost is \$8,123.00

PRESSURE SWING ABSORPTION UNIT

REACTION VESSELS

STORAGE TANKS

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BELOW AVERAGE

**Below Average Student Original Graded Assignment on Final Project
Report**

Production of Ethylene from Ethanol

Senior Design & Professionalism II

Final Report

Submitted by:

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Ryan Livingston

Rafid Matti

Reema Matti

To:

Dr. Emmanuel Dada

Department of Chemical Engineering

College of Engineering

Prairie View A&M University

Roy G College of engineering

May 3, 2021

78%
|

LETTER OF TRANSMITTAL

December 13, 2021

Department of Chemical Engineering Prairie View A&M University
100 University Dr.
Prairie View, TX 77446

Dear Dr. Emmanuel Dada,

The file below is our fall 2021 senior Design & Professionalism final report. The report contains the design plant for Production of Ethylene from Ethanol project. In the report we have covered the following sections: project scope, project planning and task identification, Literature review, process selection, process description, material and energy balances, discussion, conclusions and recommendations, references, appendix, and sample calculations. In addition, our selected method to produce Ethylene from Ethanol is also included in this report.

Our group selected the Catalytic Dehydrogenation of Ethanol method to produce Ethylene from Ethanol. In the catalytic dehydration of ethanol to form ethylene, an acid catalyst first protonates the hydroxyl group, which leaves as a water molecule. The conjugate base of the catalyst then deprotonates the methyl group, and the hydrocarbon rearranges into ethylene.

Finally, the first half of the design is done, we will look forward to completing the second half of our design with attention. Our team will make improvements to our design as requested by the evaluators and the instructors.

OK

Sincerely,

Alexus Lovelace
Ryan Livingston
Rafid Matti
Reema Matti

ACKNOWLEDGEMENT

Our group would like to acknowledge Dr. Emmanuel Dada and Dr. Lealon Martin for their assistance and guidance throughout the duration of the project.

PROJUCR SUMMARY

The project aims to design a plant that produces high purity ethylene from ethanol through catalytic dehydrogenation of ethanol. Through proper research we can develop the entire production of an ethylene plant. The United States is looking in to providing more chemical plants within our country. So, our plant will be in the western region of the United States (North Dakota). Using our available raw material, we will be able to safely store and produce ethylene and its side products, including wastewater. In addition to this, a detailed economic analysis will also be carried out to check the economic viability of the process. Followed by a detailed layout of our design and the mathematical calculations.

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1. Project Scope

1.1 Problem statement

By designing this project, we have many objectives to complete. When it comes to making a profitable design, we must develop proper research into the supply and demand of our raw materials. Along with supply and demand, safety is a major part of our portfolio. We must meet state regulations, follow codes, and stay within legal limits to work. Going forward into operation we must find our plant capacity. How much can our plant produce a year? Is this plant built to last 20-30 years? And identify what industry will be in. After keeping a plant capacity, we can scale backwards and calculate our feed streams, screen our reaction routes, choose a proper reactor, and start to produce ethylene from ethanol with the proper use of our chemical engineering background.

The project deals with some design constraints on operating conditions of the product reaction. Since, process involves an equilibrium reaction of ethanol dehydrogenation, conditions should be selected such that reaction is always favorable in forward direction. Additionally, catalysts should also contribute to making forward direction reaction even faster. In addition to this, ethanol and ethylene are highly dangerous chemicals, therefore, there should be practical preventive measures for these chemicals in the process and these measures should not be underestimated.

Ethylene is one of the most consumed chemicals across the globe and its demand is increasing day by day as it is used in the manufacture of a quite common and well-known plastic which is polyvinyl chloride (PVC). PVC is used in many applications including pipelines and construction market. About 70% of the construction market of the world is using PVC and therefore, ethylene demand is increasing with an increase of 3.5% each year. In the perspective of manufacturing technique, catalytic dehydration consumes less amount of energy than that of naphtha cracking which is highly energy intensive. Therefore, this project is of great significance not only because it is product a highly valuable chemical, but also because it involves a less energy intensive process in its manufacturing.

1.2 Client identification and recognition of need

Ethylene is a major raw material to manufacture polyethylene, polyethylene terephthalate and polystyrene and polyvinyl chloride. All these materials play a vital role in synthesis of various industrial and consumer products such as packaging, transportation, textile, and construction industries.

Client 1: The largest consumer of ethylene is the polyethylene production sector and about 60% of global ethylene is used in production of polyethylene. High density polyethylene is used in pipes of water, gas, and irrigation. Additionally, low density polyethylene is used in packaging and food packaging as well [6].

Companies Names	Product
Shell Polymers	They use ethylene to manufacture polyethylene which in turn is used for piping irrigation of water and gas.

Petro Extrusion Technologies, In	They are specialized in extrusion of polyethylene to mold in specific shapes.
Chevron Corporation	Ethylene is polymerized in polyethylene to produce a wide range of plastics.
PolyOne Corporation	Produce thermoplastic materials, vinyl resins etc.

Table 1: Ethylene client list

Client 2: The next largest consumption of ethylene is the ethylene oxide production sector which is used to produce ethylene glycol. Nonethylene glycol is employed in the production of textile products, PET bottles and polyester film. It is also used as an anti-freezing agent [6].

Companies Names	Product
Twin Specialties	They use ethylene to produce ethylene glycol in both liquid and powder form.
CJ Chemicals	Provide ethylene glycol for chemical industry.
E & C Chemicals Inc.	Provide ethylene glycol in different packaging, bottler, drum, and canister.
Hibrett Poratex	Produce ethylene glycol and other cleansing materials.

Table 2: List of companies

1.3 Plant Production and Location

When it comes to selecting the proper location to produce ethylene from ethanol many factors come into play. For example, raw materials, climate conditions, availability of water, fuel and power, and the financial aspect. Production and location are primarily based on the availability of raw materials. Ethanol's raw materials are based on glucose sugars and starches like corn.

The United States is a huge consumer of ethanol and corn fields so the best option would be to state within the country. North Dakota is in the Midwest region of the United States, with exceedingly high production. Production a year for North Dakota Is 6,480,000 tons. Our location will be in this state along the Missouri river, so we have the availability of water. There are 10% sold in the state and 90% shipped. Choosing this location, we will be next to many wastewaters treatment plants to store and get rid of the excess by products that we have from our system.

Operating within North Dakota many regulations will have to be met. The seven orders act which states we cannot be within 100 feet from schools, churches, and places within that span of human life. A Constuction permit is needed to build along with following the clean air act and getting an air pollutant permit.

1.4 Contemporary issues and impact of projects on society

Ethylene is a very hazardous substance because it is a gas that can affect it when breathing. Furthermore, if it contacts the skin, it can cause frostbite. Exposure to ethylene can cause headaches, dizziness, fatigue, lightheadedness, confusion, and unconsciousness.

1.4.1 Contemporary issues relevant to project

The contemporary issues related to the process can be technical, geological, and political. The project focuses on cost-effective production of ethylene, however, there is still a need to consider the optimum process conditions for the process. In addition to this, it is necessary to focus on green sources of production of ethanol (raw material). Ethanol is being obtained from fossil fuels or syngas. There is a need to produce ethanol from green and sustainable processes using abundantly available feedstock. In the US, there is a great inclination towards production of ethanol using corn feedstock. Another inclination towards algae which does not require regeneration is an associated step with yeast to produce ethanol [7]. Aside from issues related to process, there are some other issues related to exterior circumstances. For instance, ethanol should be delivered with stringent conditions and proper storage because it can be evaporated. Moreover, pressure inside the storage vessel should also be adjusted to avoid bursting. In addition to this, the weather should also be considered. Pandemic and deadly viruses can cause problems related to shipping, transportation, processing and delivering the product. Not only this, but it can also cause a halting of the operational activities in the production sector. Political instability in the region can also cause harm to industry and its production rate. The situation would be worse if political stability could slow down the pace of progress in the developing phase of the project.

1.4.2 Potential impact of project on society

Moreover, dehydrogenation of ethanol involves an intensive step of furnace which requires fuel for burning. Therefore, burning of this fuel will be detrimental to the environment as there will be considerable emissions of carbon dioxide and NO_x. There would be possibility of presence of sulfur in the fuel which will produce Sox and will cause acid rain when it mixes with atmospheric air [7]. If coal is used instead of natural gas in furnace, there would be emission of metal emission which adds ecotoxicity into air and it can make air carcinogenic for the community. Moreover, volatile organic matter being emitted can cause pathogenic smog and it may disturb the season timeline. As mentioned in previous section, exterior conditions like weather and pandemics can affect the performance of process, it can also affect society. The employees of the company can lose their jobs and others have a reduction in their performance efficiency because of lack of power. The effluents from the process can also pollute water and land of the nearby areas. This would result in the spread of diseases and contaminated food and water supply to residents. It can be sorted out by having effluent and water treatment facilities in the industry. In worst case scenario, production facilities near a shore can also cause harm to aquatic life in addition to human life.

1.5 Project constraints

Ethylene is a highly flammable chemical, one of the biggest constraints of the project is ignition; therefore, it should be kept away from heat, hot surface, open flames because they will cause ethylene to ignite.

2. Project Planning and Task Identification

2.1 Task identification

Our team was able to break down the main tasks into three sections: Topic Selection & Literature Research, Simulation Process, and Final Report. Gantt Chart is also being used to break down the main tasks and their appropriate compilation periods.

2.2 Timelines

A. Literature Search and Process Selection (1.5 months)

- a. Process Selection
 - i. Different Production Routs
 - ii. Overview of manufacture of xyz
- b. Research
 - i. Physical and chemical properties
 - ii. Handling, storage, and safety
 - iii. EPA, OSHA regulations and environmental impact
 - iv. Uses of the product
 - v. Product specification
- c. Defining process Conditions and Design Basis
 - i. Define the Plant capacity, Raw Materials, Utilities available at battery Limits, Pressure Drop for Process Streams, Ambient Conditions
 - ii. Define temperature, pressure, catalyst, and process description

B. Flow Sheet Development (3 weeks)

- a. Material and Energy Balance
 - i. Energy Balance and Basic calculations
 - ii. Process block diagram
 - iii. Material Balance around each unit, and degree of freedom analysis
 - iv. Assumptions and use of heuristics
 - v. Overall material balance with process streams
- b. Process Flow Diagram
 - i. Equipment's / process flow lines
 - ii. Equipment's numbering, naming, utility designations
 - iii. Temperature, pressure of the equipment's, volumetric and molar flow rates
 - iv. Summary of Material and energy balances
- c. Simulation Process (ASPEN/ HYSYS)
 - i. Selection of the Fluid package
 - ii. Equipment selection and process diagram, process data
 - iii. ASPEN/ HYSYS report

C. Final Report (3 months)

- a. Project Report
 - i. Letter of transmittal, acknowledgement, and project Summary
 - ii. Project Scope, project Planning, task Identification, Literature review, Process selection, process description, and material and energy balances
 - iii. Discussion, conclusions, and recommendations
 - iv. References, appendix, table of contents
- b. Power Point
- c. ASPEN/HYSYS Report

2.3 Gantt chart

The following Figure illustrates the project schedule, and the breakdown of the major tasks and sub tasks with completion predictions estimation. The Gantt chart was made in Microsoft Excel at the beginning of the semester to plan our project; it enabled our team to anticipate deadlines and complete them on time.

Gantt Chart

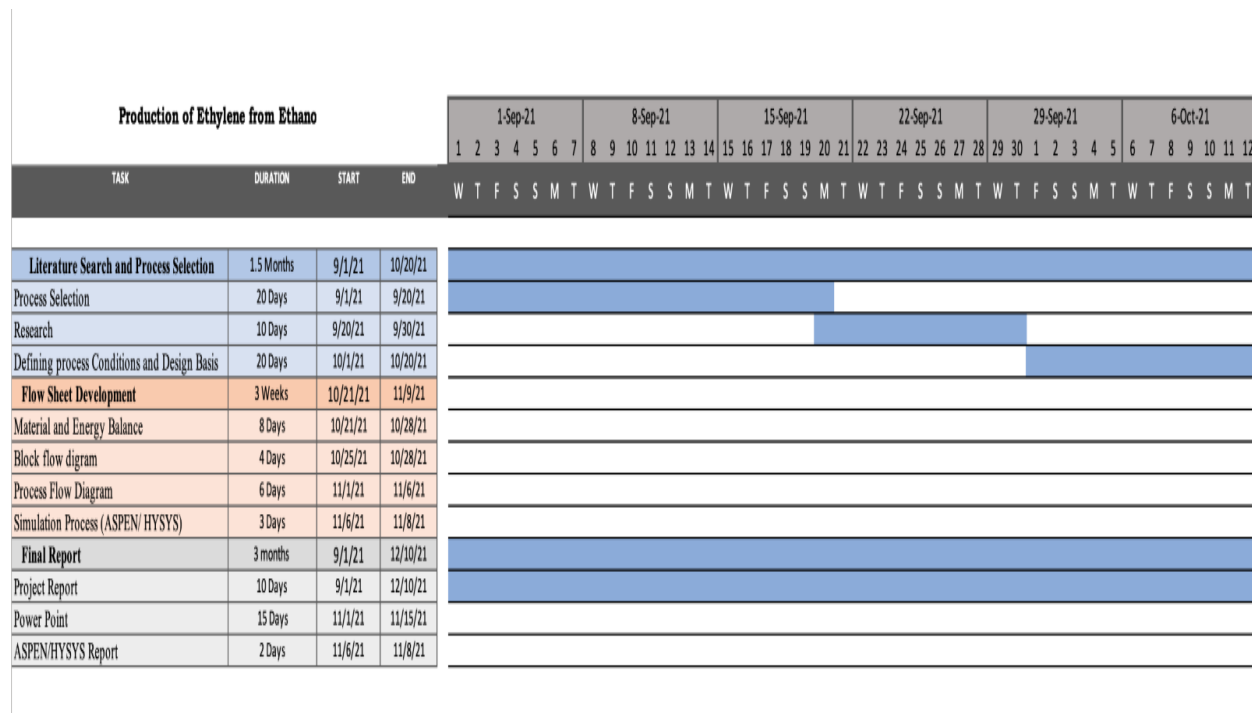


Figure 1: fall 2021 Gantt Chart

Production of Ethylene from Ethanol

Project Start:

Mon, 1/24/2022

Display Week:

1

TASK	PROGRESS	START	END	ASSIGNED TO	DURATION
Process Flow Diagram (PFD)					
ASPEN/HYSYS Simulation of Process	100%	1/24/22	2/9/22	ALL	2.5 WEEKS
Major Equipments Calculations	100%	2/9/22	3/2/22	ALL	5 WEEKS
Design of Major Equipment	100%	2/16/22	3/2/22	ALL	2 WEEKS
Equipments Specification	100%	2/21/22	3/2/22	ALL	2 WEEKS
Financial Analysis	100%	3/14/22	4/2/22	ALL	3 WEEKS
Safety and HAZOP Analysis					
HAZID	100%	3/15/22	3/19/22	ALL	5 DAYS
Hazard and Operability Study (HAZOP)	100%	3/14/22	4/2/22	ALL	3 WEEKS
Layers of Protection Analysis (LOPA)	100%	3/26/22	3/29/22	ALL	4 DAYS
Reporting					
Final Report	100%	1/24/22	4/2/22	ALL	4 MONTHS
Final Presentation	100%	4/3/22	4/9/22	ALL	1 WEEK
HYSYS/ASPEN Report	100%	4/9/22	4/9/22	ALL	1 DAY

Figure 2: Spring 2022 Gantt Chart

3.Literature review

3.1 Overview of manufacture of ethylene

Ethylene is widely used in the chemical industry. Ethylene is produced commercially by the steam cracking of a wide range of hydrocarbon feedstocks. In Europe and Asia, ethylene is obtained mainly from cracking naphtha, gasoil, and condensates with the coproduction of propylene C4 olefins and aromatics (pyrolysis gasoline). The cracking of ethane and propane, primarily carried out in the US, Canada, and the Middle East, has the advantage that it only produces ethylene and propylene, making the plants cheaper to construct and less complicated to operate [12].

3.2 Production routes

There are multiple routes to produce Ethylene from Ethanol: Catalytic Dehydration and Naphtha Cracking.

The Catalytic Dehydration route, Catalytic Dehydration is the most common route to produce Ethylene. In the catalytic dehydration of ethanol to form ethylene, an acid catalyst first protonates the hydroxyl group, which leaves as a water molecule [1]. The conjugate base of the catalyst then deprotonates the methyl group, and the hydrocarbon rearranges into ethylene [1]. This process operates at mild reaction conditions, normally 482~896°F and

0.01~1.8MPaG [2]. Ethanol dehydration process requires far less and around 80 equipment's [2]. Therefore, the construction cost of ethanol dehydration plant is much lower than any other processes due to the low standard construction material and less equipment required. Furthermore, ethanol dehydration process has high ethylene selectivity which leads to the more purified product, and this directly reduces the separation cost [2]. In addition, With the great breakthrough of biomass-to-ethanol technology, the raw material price of ethanol declined to a large extend, which makes the ethanol dehydration process is more feasible [2]. Ethanol dehydration process has more flexibility in terms of ethanol feedstock not only with different concentration but also various biomasses [2]. Therefore, ethanol dehydration process is much simpler and easier to control [2].

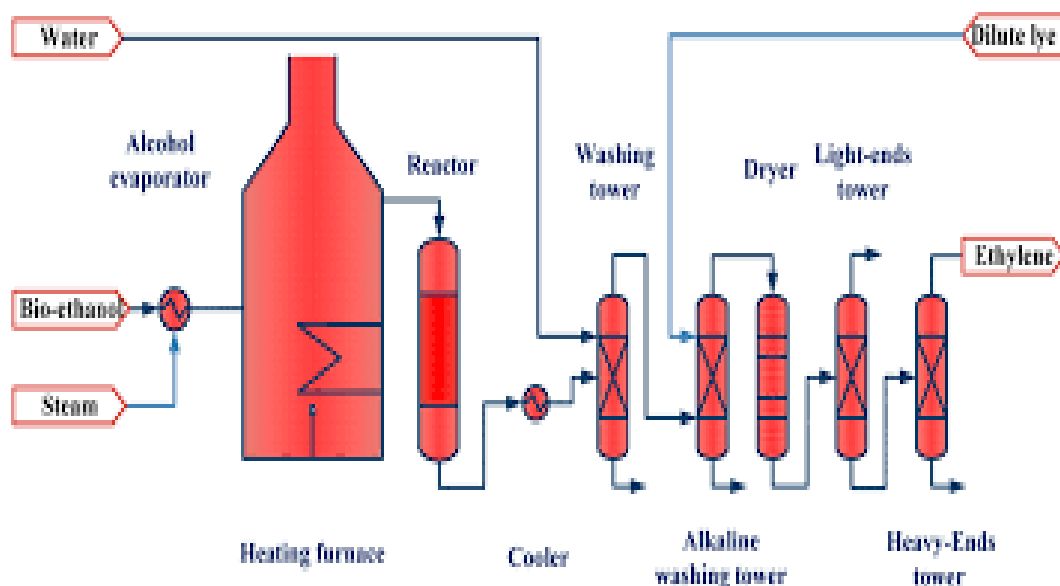


Figure 2: Catalytic Dehydration Process [10]

The Naphtha Cracking route, Naphtha is a mixture of hydrocarbons with a boiling point range of 86°F to 392°F [3]. In Naphtha cracking process, naphtha is initially heated at elevated temperature in a furnace and vaporized followed by introduction to a reactor where main reaction as well as side reaction occurs. The produced gas is then compressed and sent to the drying section. Acid gases are removed from dry stream and chilled in a chiller. After this, a process stream enters separation train where methane, ethane, ethylene, propane, propene, and higher hydrocarbons are removed in subsequent manner. Furthermore, the Naphtha cracking process is not environmentally friendly, and it involves a high cost of separation train. In addition to this, this process involves coke formation which reduces the activity of catalyst in the shorter run of the process. Coking can be avoided by diluting the process stream with steam, but it would add extra cost to the process and still coke formation cannot be completely terminated. Therefore, there has been an inclination towards ethylene production through a cheaper source.

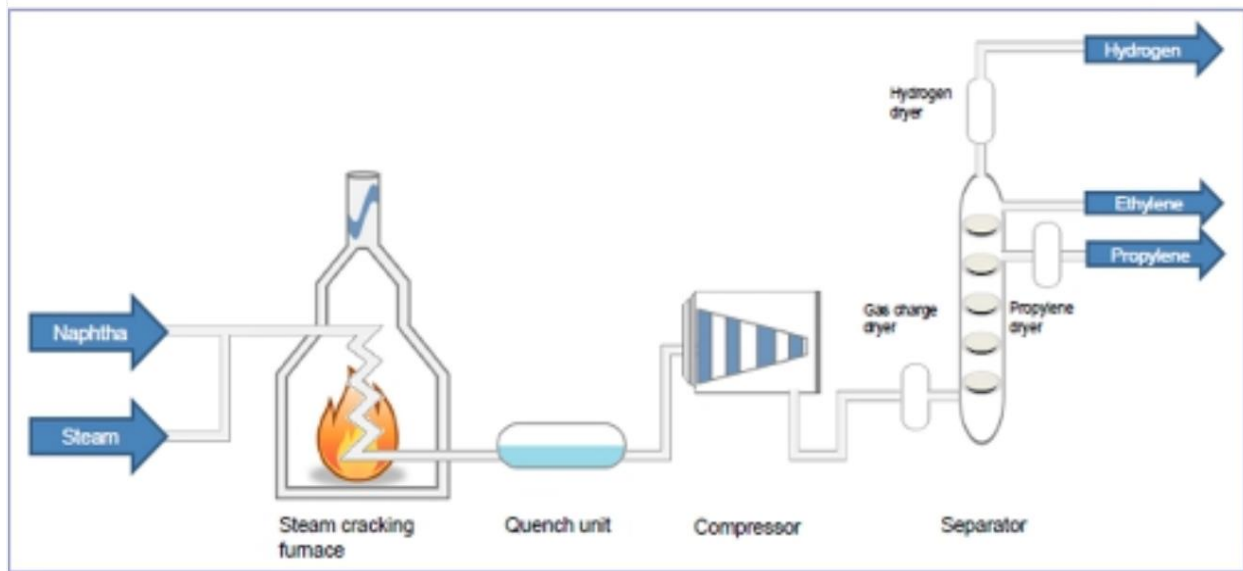


Figure 3: Naphtha Cracking process [11]

3.3 Physical and chemical properties

Ethanol is a flammable, colorless liquid with a boiling point of 173.3 °F. It has a melting point of -174.1 °F. It has a pleasant odor reminiscent of whiskey. Ethylene has a boiling point of -154.66°F, Flashpoint of -213.88°F, Ethylene is Very toxic and Highly Flammable.

Physical Properties of Ethanol

Table Title here

Properties	Data
Chemical Formula	C_2H_6O or CH_3CH_2OH
Flash Point	53.6 °F
Boiling Point	173.3 °F
Melting point	-174.1 °F
Vapor Pressure	5.95 kPa
Appearance	Colorless
Molecular Weight	46.07g /mol
Density	789 g/l
Odor	Reminiscent of whiskey

Table 3: Physical Properties of Ethanol

Physical Properties of Ethylene

Properties	Data
------------	------

Chemical Formula	C ₂ H ₄ or CH ₂ =CH ₂
Flash Point	-213.88 °F
Boiling Point	-154.66 °F
Melting point	-272.56 °F
Vapor Pressure	6.9449 kPa
Appearance	Colorless
Molecular Weight	28.05 g /mol
Density	1.260 g/l
Odor	sweet

Table 4: Physical Properties of Ethylene

Chemical Properties of Ethanol

Properties	Data
Toxicity	Very toxic
Flammability	highly flammable with a flashpoint of just 54.86 °F.
Reactivity	reacts violently with acetyl chloride and acetyl bromide
Chemical Stability	Stable under normal temperatures and pressures
Oxidation States	-1 to +1
Acidity	15.9 (H ₂ O), 29.8 (DMSO)
Heat of Combustion	1368 (kJ mol ⁻¹)
Chemical bonding	The bonds between the hydrogen and carbon atoms are nonpolar covalent bonds, The hydrogen-oxygen and carbon-oxygen bonds are polar covalent bonds.

Table 5: Chemical Properties of Ethanol

Chemical Properties of Ethylene

Properties	Data
Toxicity	Very toxic
Flammability	Highly flammable
Reactivity	the active site is the double bond for example, ethene readily undergoes addition reactions.
Chemical Stability	
Oxidation States	-2

Acidity	
Heat of Combustion	1387.4 kJ/mol
Chemical bonding	Ethene has a double bond between the carbons and single bonds between each hydrogen and carbon

Table 6: Chemical Properties of Ethylene

3.4 Handling, storage, and safety

Ethylene is a highly flammable component; it should be stored at a temperature Near 32°F. ethylene should be stored in a well-ventilated place, and the container should be tightly closed.

3.5 Handling

Ethylene should be kept away from heat, hot surface, open flames, and other ignition sources. There should be no smoking near ethylene and only non-sparking tools should be used. Moreover, explosive proof equipment should be used [4].

While handling storage tanks, leather gloves and shoes should be worn. These storage tanks should not be dragged, slide, roll or drop. There should be a removable valve cover which should be protected by a cap. Moreover, carts should be used while carrying storage tanks. There should be no instant object like a wrench to use for opening valve. It may cause damage which, in turn, will cause leakage. After each use, the tank should be closed even if it is empty. Never supply flammable material near to ethylene. An elevated temperature may cause damage to vessels and valves; therefore, storage should be done at low temperature [4].

3.6 Storage

Storage temperature should not exceed 35°F. No flame or flammable material should bring close to ethylene. Special packaging should be done to avoid natural fire according to regulations like NFPA 55. Full and empty containers should be stored separately. Protection caps should be installed when the vessel is empty. It should be stored with proper ventilation to avoid oxygen deficiency [4].

3.7 Safety

Because ethanol and ethylene are both very flammable, special care must be taken when transporting them to and from the facility, as well as when storing them. At roughly 790°F, ethanol suddenly combusts. Because the reactors operate at or near this temperature (750°F). To ensure that the temperatures in the furnaces and compressor exhaust stream never approach this level, it is critical to invest in precise and attentive controllers. Because ethylene's ignition temperature is 914°F and the plant spends most of its time in cryogenic temperatures, there is no possibility of it accidentally autoigniting. Furthermore, none of the byproducts are in any danger [4]. Ethanol is less volatile than ethylene and hence has a lower risk of causing an explosion. When converted to vapor, however, ethanol becomes very flammable and poses a bigger risk to the plant. To facilitate prompt detection of leaks, the highly concentrated ethanol reactor input stream should

be treated similarly. Another issue to consider is the spontaneous polymerization of ethylene by free radicals. On a large scale, such processes are frequently utilized to produce polyethylene. Free radical polymerization requires astronomically high pressures (about 1000atm) to occur, hence this is not a significant operational risk in this plant.

To reduce the chance of leaks, it is also a clever idea to put more money into the piping and transport equipment. If an ethylene leak goes undetected, the nearby environment will quickly surpass the lower flammability limit of ethylene in air (approximately 3%), putting the plant, the operators, and the surrounding area in grave danger [4].

3.7.1 EPA, OSHA regulations and environmental impact

Ethylene is considered a hazardous material by OSHA Hazard Communication Standard (29 CFR 1910.1200) [4]. It is a category 1 flammable gas, and it has category 3 Narcotics effect. In a single word, it is reported as “danger”. The hazard pictogram for ethylene is.



It is dangerous because it is an extremely flammable gas and even under pressure conditions, it contains gases which may explode. It can also cause dizziness and may result in frostbite. It can also replace oxygen and cause suffocation [5].

Ethylene has effects on aquatic, terrestrial and humans. For aquatic life, there is less data available, however, an old study shows that an exposure of ethylene of 22 mg/L for 1 hour causes red spots on fishes. Moreover, plants are highly susceptible to ethylene because plants produce ethylene during their growth stages which affects their fruit ripening. The exposure limit for woody and non-woody types of plants ranges from 25 mg/L to 700 mg/L [5].

For many years, ethylene has been used for anesthesia, however, high exposure can have detrimental effects on our health. Humans are usually exposed to ethylene in the air and the maximum limit estimated to be 0.05 mg/L. High exposure of ethylene can cause cancer and it also acts as a genotoxicant [5].

3.8 Uses

Ethylene is used to make manufactured plastics, antifreeze, fibers, ethylene oxide, polyethylene for plastics, alcohol, mustard gas, and other organics, among other things. It is also employed in plant growth regulator, herbicide (to accelerate the ripening of harvested fruits and vegetables,

curing agent for tobacco). Polyethylene, polypropylene, ethylene glycols, ethylene oxide, ethylene dichloride, aluminum alkyls, acetaldehyde, ethyl alcohol, polystyrene, styrene, polyvinyl chloride, SBR, polyester resin, trichloroethylene, vinyl chloride, vinyl acetate, ethyl chloride, ethylene chlorohydrin, and other materials are all manufactured from ethylene. Ethylene is used as a refrigerant, as an anesthetic, in metal welding and cutting and in fruit ripening sprays in orchards.

3.9 Product specification

Ethylene specification

Substance Name	Ethylene
Chemical Name	Ethylene
Formula	C ₂ H ₄
CAS Number	74-85-1
Other names	Ethene, Acetone, Refrigerant gas R1150
Purity	(Write purity obtained)
Auto ignition point	842°F
Density	0.974 g/cm ³

Table 7: Ethylene specification

4.Process selection

4.1 Market analysis and trends

According to Market analysis and trends ethylene market has been growing since 1990 and will continue to grow more in the future. The production of ethylene has reached 32000 thousand metric tons in the year 2019.

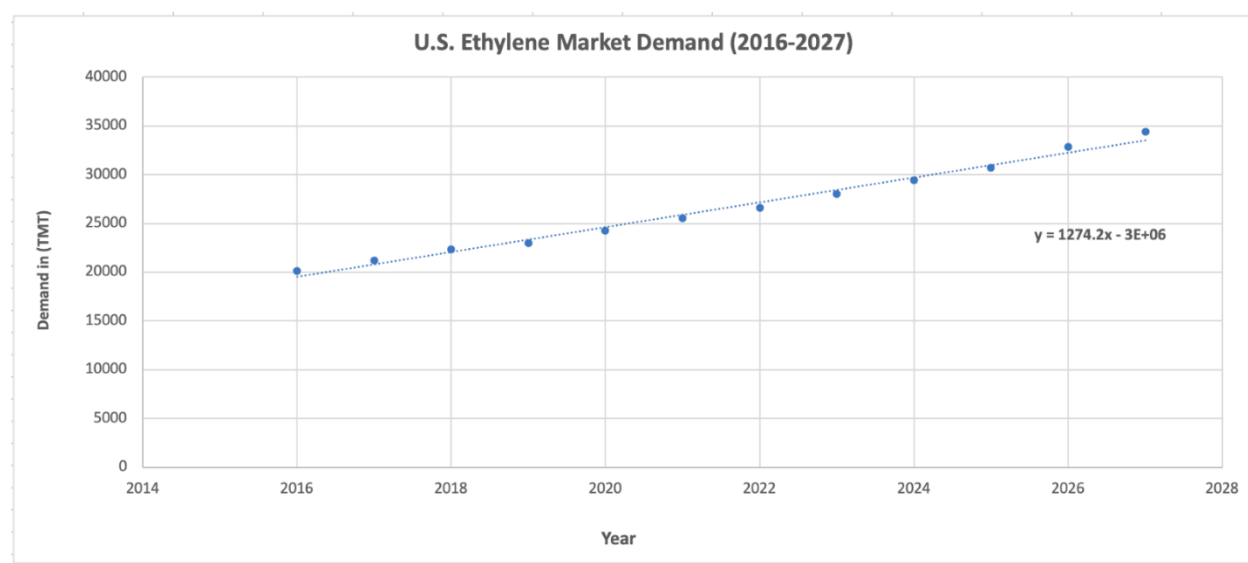


Figure 4: U.S. Ethylene production

The above figure shows the U.S. Production of Ethylene from the year 1990-2019. As seen in the year 1990, the production is nearly 16000 thousand metric tons. The production of ethylene has increased from the year 1990; and it is continuously increasing. In year 2019 the production of ethylene in U.S.A has become risen to 32000 thousand metric tons.

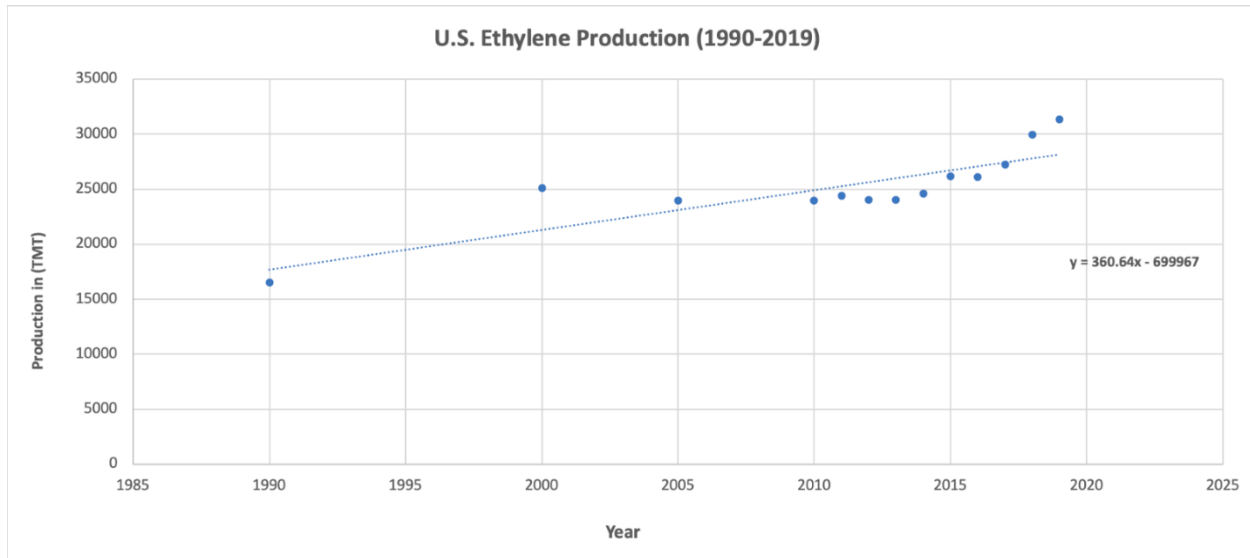


Figure 5: U.S. Ethylene Market Demand

Figure 5 illustrates the U.S. Ethylene Demand from year 2016-2027. In the year 2016 the demand was 20000 thousand metric tons. The demand of Ethylene has increased from the year 2019 to the year 2021 almost 60000 thousand metric tons, and it will continue increasing. Y is representing the tradeline equation of the U.S. Ethylene Demand.

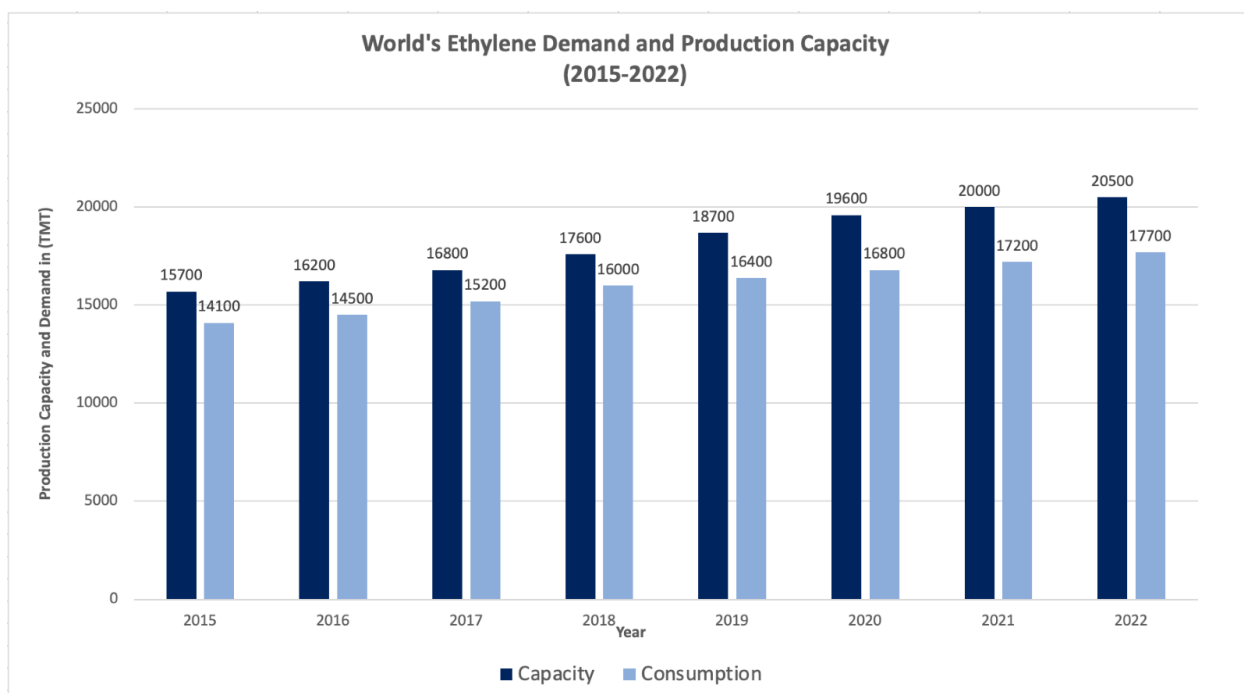


Figure 6: Worlds Ethylene Demand and Production Capacity

The figure above shows the Worlds Ethylene Demand and Capacity from the year 2015-2022. As seen on the graph above the Capacity is higher than the Consumption. In year 2015 the capacity of ethylene is around 15700 thousand metric tons, and the consumption of ethylene is 14100 thousand metric tons. The Capacity of ethylene has increased since the year 2015.

4.2 Reaction routes to producing products

4.2.1 Reaction route 1

Catalytic Dehydration is the most common route to produce Ethylene. First, an acid catalyst protonates the hydroxyl group, which leaves as a water molecule. The conjugate base of the catalyst then deprotonates the methyl group, and the hydrocarbon rearranges into ethylene. The conjugate base of the catalyst then deprotonates the methyl group, and the hydrocarbon rearranges into ethylene [1]. This process operates at mild reaction conditions, normally 482~896°F and 0.01~1.8MPaG [2]. Ethanol dehydration process requires far less and around 80 equipment's [2].

4.2.2 Reaction route 2

For naphtha cracking, first, preheated naphtha is thermally cracked in the presence of steam. Naphtha will pass through a tube of the cracking furnace, and the furnace operates at a high temperature so that the heat for the endothermic cracking reactions is provided by

the fuel combustion. The furnace consists of the radiant zone, where the cracking reaction occurs at $> 1382^{\circ}\text{F}$, and the convective zone, where the feedstock preheating takes place at up to 1202°F [13]. Now, using the transfer line heat exchanger the stream will rapidly quench. As the product contains significant amounts of heavy hydrocarbons, a primary fractionator is installed to remove tar and oily material from the cracked gases [13]. The product is further quenched to near-ambient temperature to remove the “heavies.” This is followed by a multistage compression system to raise the pressure of the lighter gaseous products to around 4 MPa [13]. An adsorption column of molecular sieves facilitates the drying, followed by a caustic wash to remove acid gases such as CO_2 [2].

4.3 Process screening using gross profit analysis

To properly perform the process screening a profit analyst was taken for multiple alternatives. The most profitable process was chosen solely based on economics and cost.

Catalytic Dehydrogenation

$\text{C}_2\text{H}_5\text{OH} \rightarrow \text{C}_2\text{H}_4 + \text{H}_2\text{O}$			
Pound- mole	1	1	1
Molecular Weight	0.1016 lb-mol	0.0612 lb-mol	0.0397 lb-mol
Pound/ Pound of Ethylene	1.64	1	.642
Cents Per Pound	26.62	19.3	0.0015

Table 8: Gross profit analysis

$$\text{Theoretical Equation} = \text{Cost (Products)} - \text{Cost (Reactants)}$$

$$9.3(1) + .642(0.0015) - 26.62(1.64) = 24.35$$

Gross Profit Analysts = 24.36 cents/ pound.

4.4 Process comparison and selection

Compression Between different routes

Method	Advantages	Disadvantages
Naphtha Cracking	· A variety of products can be formed. · Naphtha is obtained from petroleum industries i.e. raw material is abundantly available.	· Higher emission of greenhouse gases which disturb the environment. · A few side products can be formed.

	Produce ethylene in higher amounts because of cracking of various hydrocarbons.	- It might involve the separation of components through energy intensive techniques such as in separation of azeotropes. - Feed might be impure in a greater extent.
Catalytic Dehydrogenation of Ethanol	- Undesired products will be less in number compared to other techniques. - Feed will be pure in many cases, however, costly to produce. - Energy consumption will be less compared to other techniques.	- Emission of greenhouse gases, though less compared to others. - There would be sensitive separation technologies such as cryogenic distillation.

Table 9: Comparison Between different routes

We decided to go with the Catalytic Dehydrogenation of Ethanol method because it has fewer disadvantages than Naphtha Cracking process. Catalytic Dehydrogenation of Ethanol process is more environmental Safety than Naphtha Cracking process in addition to safety Catalytic Dehydrogenation of Ethanol process has a better Reaction Yield/Selectivity. We have used the following method to select which process to go with.

Process Selection

Criteria	Naphtha Cracking	Catalytic Dehydrogenation
Raw Material Availability /Cost	5	4
Reaction Yield/Selectivity	3	5
Environmental Safety	2	4
Safety/Operability	4	4
Total Score	14	17

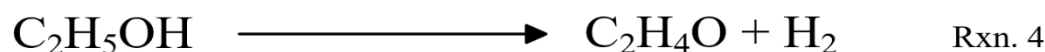
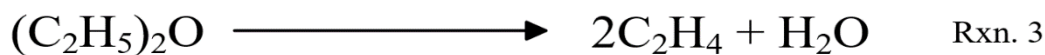
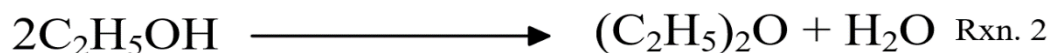
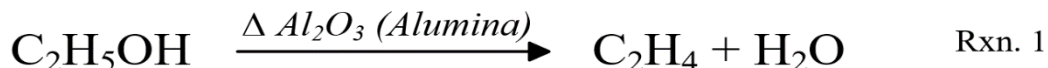
Table 10: Process Selection

Process Selection (Highest: 5 and Lowest: 1)

5. Process description

5.1 Process chemistry

The primary reaction (Rxn. 1) that drives the production of ethylene through the catalytic dehydration of ethanol can be seen below:



Because it is impossible to have 100% conversion on any reaction, side reactions will present themselves within the process. That is why it's important to understand the chemistry of the by-products involved in our catalytic dehydration process.

As previously stated, Rxn. 1 depicts the main reaction that drives our process. For every one mole of ethanol present in *Rxn. 1*, one mole of ethylene will be produced. Here, the dehydration of our alcohol, Ethanol, is sped up by the catalyst, Aluminum (III) Oxide. The alumina-based catalyst is known for providing high yield in the catalytic dehydration process.

From here, our reactor becomes host to the three side reactions also listed above. Inside *Rxn. 1*, our raw material will experience another dehydration where the –OH group is removed and produces an aqueous product, diethyl ether and water. *Rxn. 3* produces another undesired product, Acetaldehyde, through oxidation. Lastly, like *Rxn. 3*, *Rxn. 4* contributes to the overall production of our desired product, Ethylene.

5.2 Process (Block) flow diagram and process description

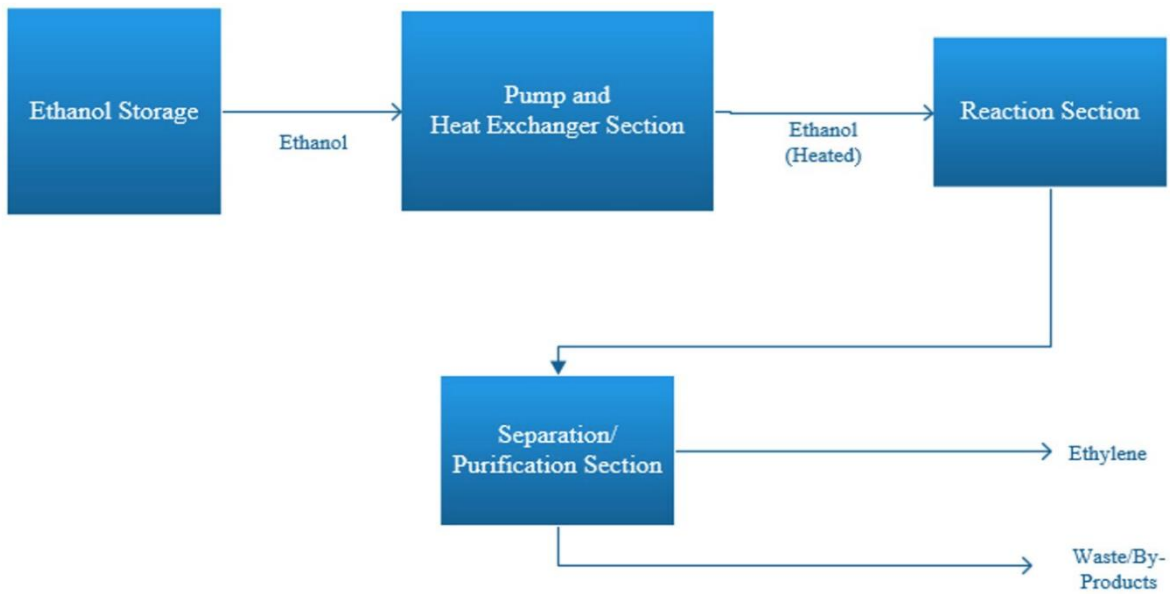


Figure 8: Block Flow Diagram

Above is the block flow diagram (BFD) for the process. Ethanol is first fed from our tank to a pump at ambient temperature (77°F) and standard pressure (14.7 psi) where the pressure is increased to 629 psi. The fluid is then transferred from the tank to the heat exchanger. From here we have our stream exiting the reactor section at approximately 629°F. From here the stream will enter the compressor to increase the pressure to our design flash pressure (653.7 psi). From here our product will enter the separation/ purification section, where we will separate our aqueous waste through flash separation and send our stream through the purifying section to get rid of the final impurities and store our high purity grade ethylene (95%).

Catalytic Dehydration of Ethanol to Ethylene

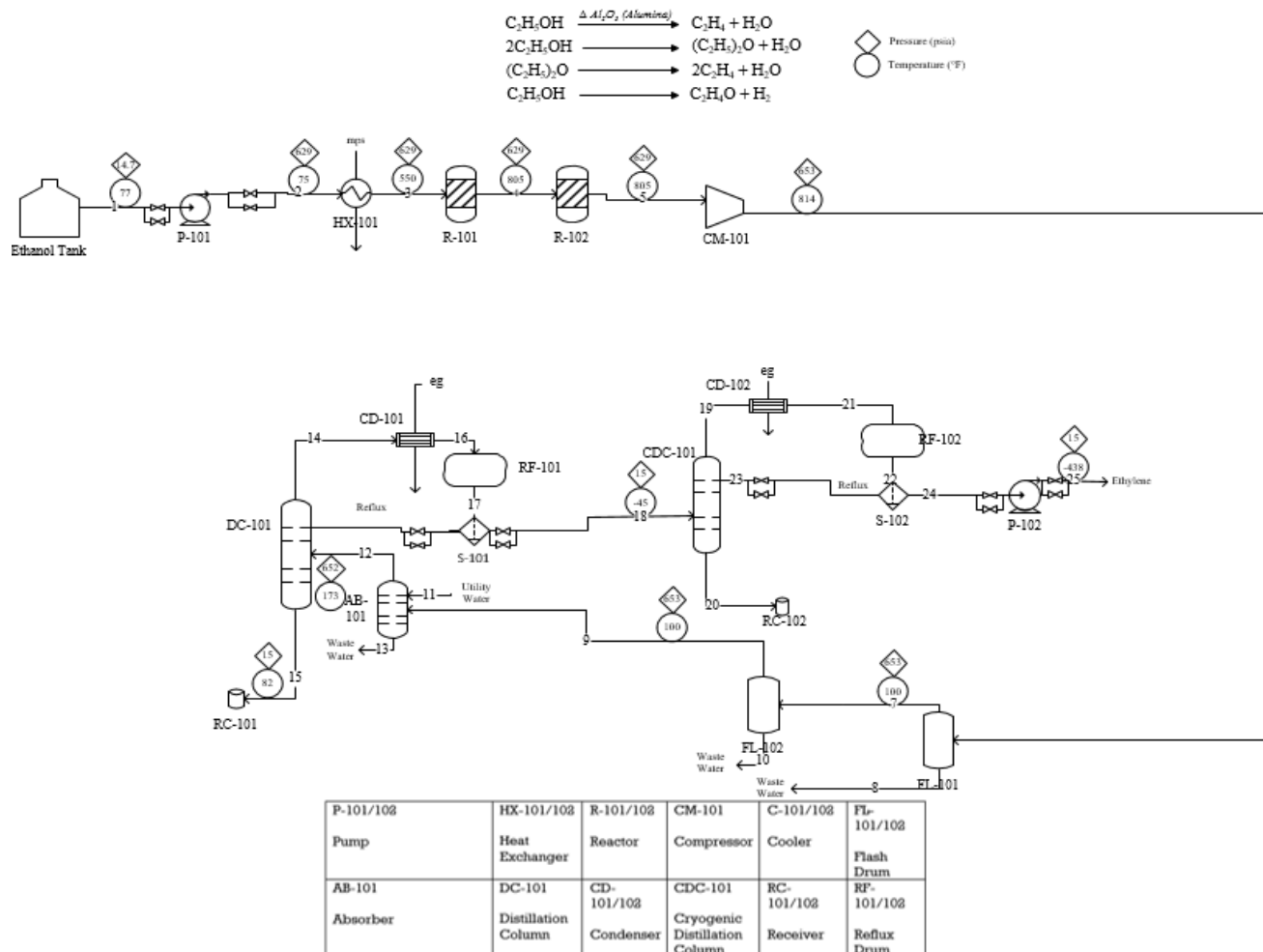


Figure 9: Process Flow Diagram

Pump (1-2)

Above is a preliminary PFD of our overall Process. From stream 1 we have our Raw material, Ethanol (95wt%), going to our pump from our tank at ambient temperature (77°F) and standard pressure (14.7 psi) where the pressure is increased to (629 psi).

Heaters, Reactors and Compressor (2-6)

From the pump our feed stream is sent through the heater to raise our feed stream to our reaction temperature (Approximately 805°F). Then we have two PBR reactors, our reactors are in series, it is an adiabatic process where there is no change in temperature across the reactors. Our product ethylene with flied imparity's will come out and it will be sent to a compressor and then to a flash separation.

Flash Separations and Absorber (6-9)

From the Compressor it will be sent to two Flash separation sections, top is going into the second flash separator and then we will sent it to absorber; we have utility water coming down and take

out some of the impurity's that we have sent from the flash separator and more wastewater is coming off the absorber.

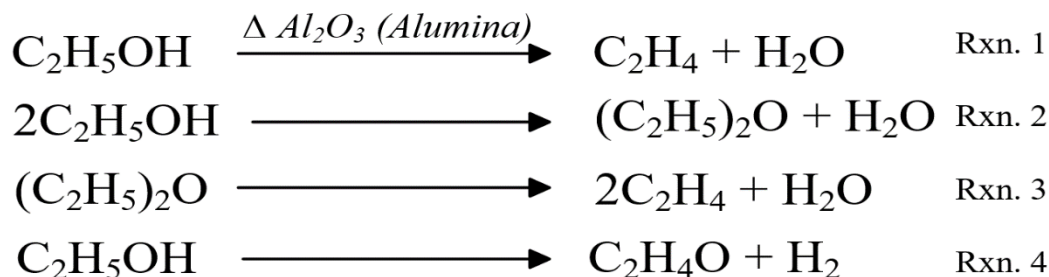
Distillation Columns, condenser, Reflex Drum, cryogenic Distillation Column (9-24)

At the Distillation column light key components will go through the condenser to make them into a liquid. We have a splitter after the reflux Stream sending it in the reflux back to distillation column, and then rest of the product going into another distillation column where the temperature begins to decrease as it goes through. The temperature should be kept below (154°F) so that it can stay in a liquid. After it goes to another distillation column, we have another splitter sending more reflux to the cryogenic distillation column and finally we have product coming out.

5.2.1 Raw material preparation

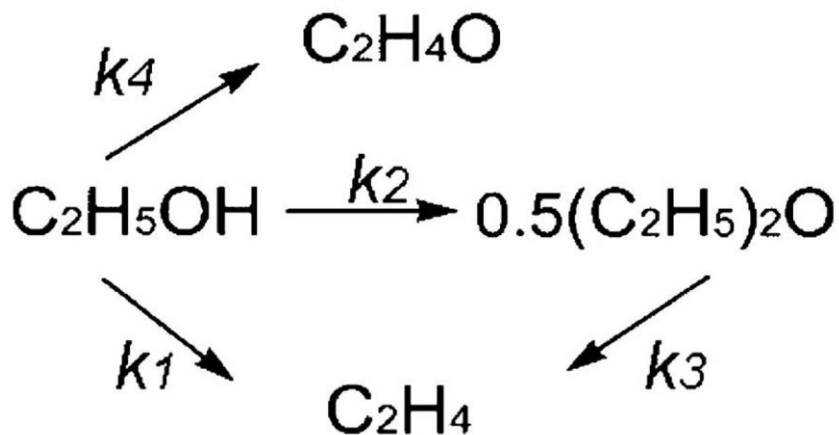
Most of the ethanol is made of corn (starches) or sugar-based predations. Aqueous solutions of ethanol will be produced through fermentation of corn. Which requires an additional catalyst or enzyme to be involved to extract. This will produce ethylene gas at a high pressure that will go back into the system as diluted water mixture and heated, forming ethanol by hydrolysis. Another way is by using dry milling or wet milling preparation. Dry milling is more compound on compound, while wet willing is more for separation of compounds into liquids using solid materials.

5.2.2 Reaction and reactor operation



Reactor Operation Fixed packed bed reactor. This reactor is one of the many reactors used in chemical processes. It is used for stripping, absorption, and catalytic reactions. The process is as follows: in a fixed bed reactor the catalyst is located within the tube and is then reacted with the reactants to produce the products.

5.2.2 Reaction Network



5.2.3 Separations

Three Flash Drum separators are being used throughout this process. The heated liquid stream flows into the separator through a valve. This causes the pressure to be reduced causing them to start to partially vaporize. An absorber is used to purify the products coming out of the flash drum. While the distillation columns separate the products from the wastewater.

5.2.4 Product to storage

Our reaction has many elements where wastewater is being produced. For this reason, we will be located next to many wastewater plants so that we are able to distribute our wastewater instead of keeping it inside of the plant. However, small traces of our side products will be found within the water itself.

6. Material and Energy Balances

6.1 Basis of calculations

The following material balance was based off literature received on the largest Ethylene plants in production.

We expect to produce .2MT (400,000 lbs./yr.) per annum according to the following calculations.

After establishing our plant capacity, we performed the following dimensional analysis to get our product stream:

$$F_{BF} = 400,000 \frac{\text{lbs.}}{\text{yr.}} * \left(\frac{1 \text{ yr.}}{365 \text{ days}} \right) * \left(\frac{1 \text{ day}}{24 \text{ hours}} \right) = 45,662.10 \frac{\text{lbs.}}{\text{hr.}} \cong 46,000 \frac{\text{lbs.}}{\text{hr.}}$$

Now we can use the following algorithm to calculate the amount of Ethanol being consumed during the process:

$$\left(\frac{1 \text{ mol } C_2H_5OH}{1 \text{ mol } C_2H_4}\right) * \left(\frac{1 \text{ mol } C_2H_4}{.062 \frac{\text{lb.}}{\text{mol}} C_2H_4}\right) * \left(45,662.1 \frac{\text{lbs.}}{\text{hr.}}\right) * \left(\frac{.1 \frac{\text{lb.}}{\text{mol}} C_2H_5OH}{1 \text{ mol } C_2H_4}\right)$$

$$= 73,648.55 \frac{\text{lb.}}{\text{hr.}} C_2H_5OH$$

With the conversion rate we received through literature review, we can now calculate the initial flow rate of Ethanol into our system.

$$F_{Ai} = \frac{\text{EtOH consumption}}{\text{EtOH conversion}} = \frac{73,648.55 \frac{\text{lbs.}}{\text{hr.}}}{.95} \cong 77,525 \frac{\text{lbs.}}{\text{hr.}}$$

6.1.2 Material Balance around major and supporting equipment

Unit:(R-101) Reactor (MEB)

1) Mole Balance

$$\frac{dF_A}{dW} = r'_A$$

$$\frac{dF_B}{dW} = r'_B$$

$$\frac{dF_C}{dW} = r'_C$$

$$\frac{dF_D}{dW} = r'_D$$

$$\frac{dF_E}{dW} = r'_E$$

$$\frac{dF_F}{dW} = r'_F$$

2) Rate Laws

Rates of Formation

$$\sum r_A = r_{1A} + r_{2A} + r_{4A}$$

$$\sum r_B = r_{1B} + r_{3B}$$

$$\sum r_C = r_{1C} + r_{2C} + r_{3C}$$

$$\sum r_D = r_{2D} + r_{3D}$$

$$\sum r_E = r_{4E}$$

$$\sum r_F = r_{4F}$$

Relative Rates

$$\frac{r_{1A}}{-1} = \frac{r_{1B}}{1} = \frac{r_{1C}}{1}; -r_{1A} = r_{1B} = r_{1C}$$

$$\frac{r_{2A}}{-2} = \frac{r_{2D}}{1} = \frac{r_{2C}}{1}; -2r_{2A} = r_{2D} = r_{2C}$$

$$\frac{r_{3D}}{-1} = \frac{r_{3B}}{2} = \frac{r_{3C}}{1}; -r_{3D} = r_{3B} = r_{3C}$$

$$\frac{r_{4A}}{-1} = \frac{r_{4E}}{1} = \frac{r_{4F}}{1}; -r_{4A} = r_{4E} = r_{4F}$$

Net Rate Laws based on Rates of Formation

$$r_A = k_1 C_A + k_2 C_A^2 + k_4 C_A$$

$$r_B = k_1 C_A + k_3 C_D^2$$

$$r_C = k_1 C_A + k_2 C_A + k_3 C_D$$

$$r_D = k_2 C_A^2 + k_3 C_D$$

$$r_E = k_4 C_A$$

$$r_F = k_4 C_A$$

Rate Constant (k_j) calculations

$$k_j = A_j e^{\left(\frac{-E_{aj}}{RT}\right)} \text{ Parent Function}$$

$$k_1 = (5.41 * 10^6) e^{\left(\frac{-147.7 * 10^3 \frac{J}{mol}}{\left(8.314 \frac{J}{mol * K}\right) * (702.92K)}\right)} = 5.716 * 10^{-5}$$

$$k_2 = (9.55 * 10^7) e^{\left(\frac{-101.0 * 10^3 \frac{J}{mol}}{\left(8.314 \frac{J}{mol * K}\right) * (702.92K)}\right)} = 2.980$$

$$k_3 = (2.79 * 10^{10}) e^{\left(\frac{-135 * 10^3 \frac{J}{mol}}{\left(8.314 \frac{J}{mol * K}\right) * (702.92K)}\right)} = 2.589$$

$$k_4 = (2.78 * 10^8) e^{\left(\frac{-138.4 * 10^3 \frac{J}{mol}}{(8.314 \frac{J}{mol * K}) * (702.92 K)} \right)} = 1.442 * 10^{-2}$$

3) Stoichiometry

$$C_j = C_{To} \frac{F_j T_o P}{F_T T P_o} \text{ Recall from Kinetics}$$

$$C_A = C_{To} \frac{F_A T_o P}{F_T T P_o}$$

$$C_D = C_{To} \frac{F_D T_o P}{F_T T P_o}$$

4) Combine

$$\frac{dF_A}{dW} = r'_A = - \left[k_1 k_4 \left(C_{To} \frac{F_A T_o P}{F_T T P_o} \right) k_2 \left(C_{To} \frac{F_A T_o P}{F_T T P_o} \right)^2 \right]$$

$$\frac{dF_D}{dW} = r'_D = - \left[k_2 \left(C_{To} \frac{F_A T_o P}{F_T T P_o} \right)^2 + k_3 \left(C_{To} \frac{F_D T_o P}{F_T T P_o} \right) \right]$$

5) Energy Balance

$$\frac{dT}{dW} = \frac{r'_A H_{RX}(T) - \frac{Ua}{\rho_b} (T - T_a)}{\sum F_i C_{pi}}$$

- $r'_A = - \left[k_1 k_4 \left(C_{To} \frac{F_A T_o P}{F_T T P_o} \right) k_2 \left(C_{To} \frac{F_A T_o P}{F_T T P_o} \right)^2 \right] / \rho_b$
- $H_{RX}(T) = -119.346 \frac{Btu}{lb * mol}$
- $Ua = (3.3288 * 10^6 \frac{Btu}{h * R})$
- $\rho_b = 34 \frac{lbs}{ft^3}$

The following algorithm was developed to derive the concentrations for the two reactions that drive the production of the desired product, *Rxn. 1 and Rxn. 3*. By plugging this algorithm into POLYMATH, we were able to derive the following.

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	W	0	0	100.	100.
2	Fa	4.566E+04	4.555E+04	4.566E+04	4.555E+04
3	Fb	0	0	0.0343485	0.0343485
4	Fc	0	0	225.252	225.252

5	Fd	0	0	112.5751	112.5751
6	Fe	0	0	0.1520205	0.1520205
7	Ff	0	0	0.1520205	0.1520205
8	T	77.	77.	900.	900.
9	Ft	4.566E+04	4.566E+04	4.589E+04	4.589E+04
10	k4	0.01442	0.01442	0.01442	0.01442
11	k3	2.589	2.589	2.589	2.589
12	P1	619.7	619.7	619.7	619.7
13	Ctbo	0	0	0	0
14	Ctao	0.95	0.95	0.95	0.95
15	rhob	34.	34.	34.	34.
16	Cto	0.95	0.95	0.95	0.95
17	To	77.	77.	77.	77.
18	k1	5.716E-05	5.716E-05	5.716E-05	5.716E-05
19	k2	2.98	2.98	2.98	2.98
20	Po	14.	14.	14.	14.
21	Ca	42.05107	3.57119	42.05107	3.57119
22	Cd	0	0	0.0088262	0.0088262
23	rbprime	7.07E-05	1.966E-05	0.0006781	0.0006781
24	rcprime	309.9714	2.236273	309.9714	2.236273
25	raprime	-155.0036	-155.0036	-1.119318	-1.119318
26	reprime	0.0178346	0.0015146	0.0178346	0.0015146
27	r1a	-0.0024036	-0.0024036	-0.0002041	-0.0002041
28	r1b	0.0024036	0.0002041	0.0024036	0.0002041
29	r2a	-5269.512	-5269.512	-38.00512	-38.00512
30	rdprime	154.9856	1.117126	154.9856	1.117126
31	r3d	0	-0.022851	0	-0.022851
32	r2d	-1.054E+04	-1.054E+04	-76.01024	-76.01024
33	r1c	0.0024036	0.0002041	0.0024036	0.0002041
34	r2c	-1.054E+04	-1.054E+04	-76.01024	-76.01024
35	r3b	0	0	0.022851	0.022851
36	r4a	-0.6063765	-0.6063765	-0.0514966	-0.0514966
37	r4e	0.6063765	0.0514966	0.6063765	0.0514966
38	r4f	0.6063765	0.0514966	0.6063765	0.0514966
39	Ta	900.	900.	900.	900.
40	r3c	0	0	0.022851	0.022851
41	Hr1a	-119.346	-119.346	-119.346	-119.346
42	rfprime	0.0178346	0.0015146	0.0178346	0.0015146
43	C1	0.2868647	0.024362	0.2868647	0.024362
44	Cpa	0.614	0.614	0.614	0.614
45	Cpb	0.365	0.365	0.365	0.365
46	Cpc	1.	1.	1.	1.

47	Cpd	0.0285	0.0285	0.0285	0.0285
48	Cpe	0.0114	0.0114	0.0114	0.0114
49	Cpf	3.42	3.42	3.42	3.42
50	Ua	7.403E+10	7.403E+10	7.403E+10	7.403E+10
51	HE	-1.792E+12	-1.792E+12	3.62E+05	8209.016

Due to the process downsize, our results were incorrect. However, if our circumstances were allowed to remain the same, the following results above is what would be expected.

6.1.2 Assumptions and use of heuristics

Heuristics is a mental process that is used dilly for people to solve problems and make judgments quickly and efficiently. These rule-of-thumb tactics reduce decision-making time and enable people to perform without continually pausing to consider their next move. However, heuristics is helpful to make decisions faster.

6.1.3 Overall material balance with process streams

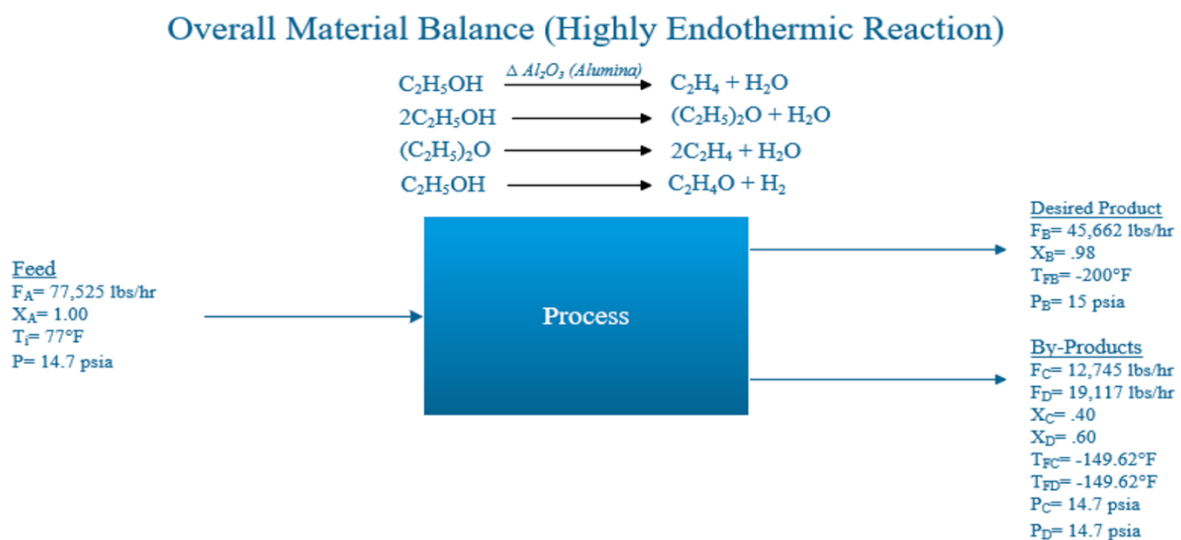


Figure 10: Overall Material Balance

Material Streams																			
Stream Name	Units	2	3	5	6	7	11	12	22	ETHANOL	ETHYLENE	RC-101	RC-102	S1	S3	S5	W	WASTE	WASTE
Description																			
From		B1	B4	B3		B3	B6	B7	B11		B14	B11	B14	B15	B2	B8	B2	B8	B7
To		B3	B6		B3	B4	B7	B2	B14	B1		B15	B15		B8	B11			
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase			Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	F	79.7481	805	718	900	549.843	813.868	100	-45.3753	77	-438.339	81.7953	-149.62	-140.117	100	172.833	100	172.833	100
Pressure	psia	628.696	628.696	639	639	628.696	653	653	14.7	14.7	14.7	14.7	14.7	14.7	653	652	653	652	653
Volume Flow	cuft/hr	1558.63	64780.2	454626	542414	23128.6	62807.2	9615.29	434608	1555.19	550.953	159.769	368.37	31366.9	9540.32	13320.3	1.44277	214.94	395.279
Vapor Phase																			
Enthalpy Flow	Btu/hr		-1.05E+08	-2.47E+09	-2.42E+09	-1.57E+08	-1.05E+08	2.04E+06	2.21E+07					2.80E+06	1.84E+07	1.35E+07			
Mass Flows	lb/hr		77525	448000	448000	77525	77525	53412.4	37717					3826.14	31553.7	45221.1			
C2H5OH	lb/hr		3876.25	0	0	77525	3876.25	3474.89	8.47E-06					0.000377443	171.498	1393.3			
C2H4	lb/hr		33990.4	0	0	0	33990.4	33988	32666.9					3823.37	27721.2	32666.9			
H2O	lb/hr		23646.6	0	0	0	23646.6	88.4068	0					0	0	0			
C2H4O	lb/hr		8154.59	0	0	0	8154.59	8003.94	4522.36					2.46992	2068.16	5920.66			
DIETH-01	lb/hr		7484.03	0	0	0	7484.03	7484.03	155.832					0.301071	1224.17	4868.37			
STEAM	lb/hr		0	448000	448000	0	0	0	0					0	0	0			
H2	lb/hr		373.156	0	0	0	373.156	373.149	371.903					0	368.613	371.903			
Mass Fractions																			
C2H5OH			0.05	0	0	1	0.05	0.0650577	2.25E-10					9.86E-08	0.00543513	0.0308108			
C2H4			0.438444	0	0	0	0.438444	0.636331	0.866106					0.999276	0.878542	0.722381			
H2O			0.305019	0	0	0	0.305019	0.00165517	0					0	0	0			
C2H4O			0.105187	0	0	0	0.105187	0.149852	0.119902					0.000645538	0.0655443	0.130927			
DIETH-01			0.096537	0	0	0	0.096537	0.140118	0.00413162					7.87E-05	0.0387965	0.107657			
STEAM			0	1	1	0	0	0	0					0	0	0			
H2			0.00481336	0	0	0	0.00481336	0.00698619	0.00986035					0	0.0116821	0.0082241			

Table 11: Material and Enthalpy Streams- Gas Phase

Material Streams																			
Stream Name	Units	2	3	5	6	7	11	12	22	ETHANOL	ETHYLENE	RC-101	RC-102	S1	S3	S5	W	WASTE W	WASTE W A
Description																			
From		B1	B4	B3		B3	B6	B7	B11		B14	B11	B14	B15	B2	B8	B2	B8	B7
To		B3	B6		B3	B4	B7	B2	B14	B1		B15	B15		B8	B11			
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase			Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	F	79.7481	805	718	900	549.843	813.868	100	-45.3753	77	-438.339	81.7953	-149.62	-140.117	100	172.833	100	172.833	100
Pressure	psia	628.696	628.696	639	639	628.696	653	653	14.7	14.7	14.7	14.7	14.7	14.7	653	652	653	652	653
Volume Flow	cuft/hr	1558.63	64780.2	454626	542414	23128.6	62807.2	9615.29	434608	1555.19	550.953	159.769	368.37	31366.9	9540.32	13320.3	1.44277	214.94	395.279
Liquid Phase																			
Enthalpy Flow	Btu/hr	-2.01E+08								-2.01E+08	7.49E+06	-1.22E+07	1.51E+06	-1.35E+07	-1.86E+07		-604715	-9.78E+06	-1.62E+08
Mass Flows	lb/hr	77525								77525	22445	7504.11	15272	18949.9	21770.3		88.4068	8102.87	24112.6
C2H5OH	lb/hr	77525								77525	3.65E-24	1393.3	8.47E-06	1393.3	3303.39		0	2081.59	401.363
C2H4	lb/hr	0								0	22073.1	4.19E-10	10593.8	6770.39	6266.72		0	1321.08	2.42031
H2O	lb/hr	0								0	0	0	0	0	0		88.4068	0	23558.2
C2H4O	lb/hr	0								0	2.93E-06	1398.29	4522.37	5918.19	5935.78		0	2083.29	150.651
DIETH-01	lb/hr	0								0	1.16E-11	4712.52	155.832	4868.05	6259.86		0	2615.67	0.00116752
STEAM	lb/hr	0								0	0	0	0	0	0		0	0	0
H2	lb/hr	0								0	371.903	4.54E-25	2.01E-22	0	4.53614		0	1.24621	0.0066246
Mass Fractions																			
C2H5OH	1									1	1.63E-28	0.185671	5.55E-10	0.0735251	0.151738		0	0.256895	0.0166454
C2H4	0									0	0.983431	5.59E-14	0.693674	0.357278	0.287857		0	0.163039	0.000100375
H2O	0									0	0	0	0	0	0		1	0	0.977006
C2H4O	0									0	1.31E-10	0.186337	0.296122	0.312307	0.272655		0	0.257105	0.00624783
DIETH-01	0									0	5.19E-16	0.627992	0.0102038	0.25689	0.287541		0	0.322807	4.84E-08
STEAM	0									0	0	0	0	0	0		0	0	0
H2	0									0	0.0165695	6.05E-29	1.32E-26	0	0.000208364		0	0.000153799	2.75E-07

Table 12: Material and Enthalpy Streams- Liquid Phase

7. PLUS/ASPEN Simulation of Process

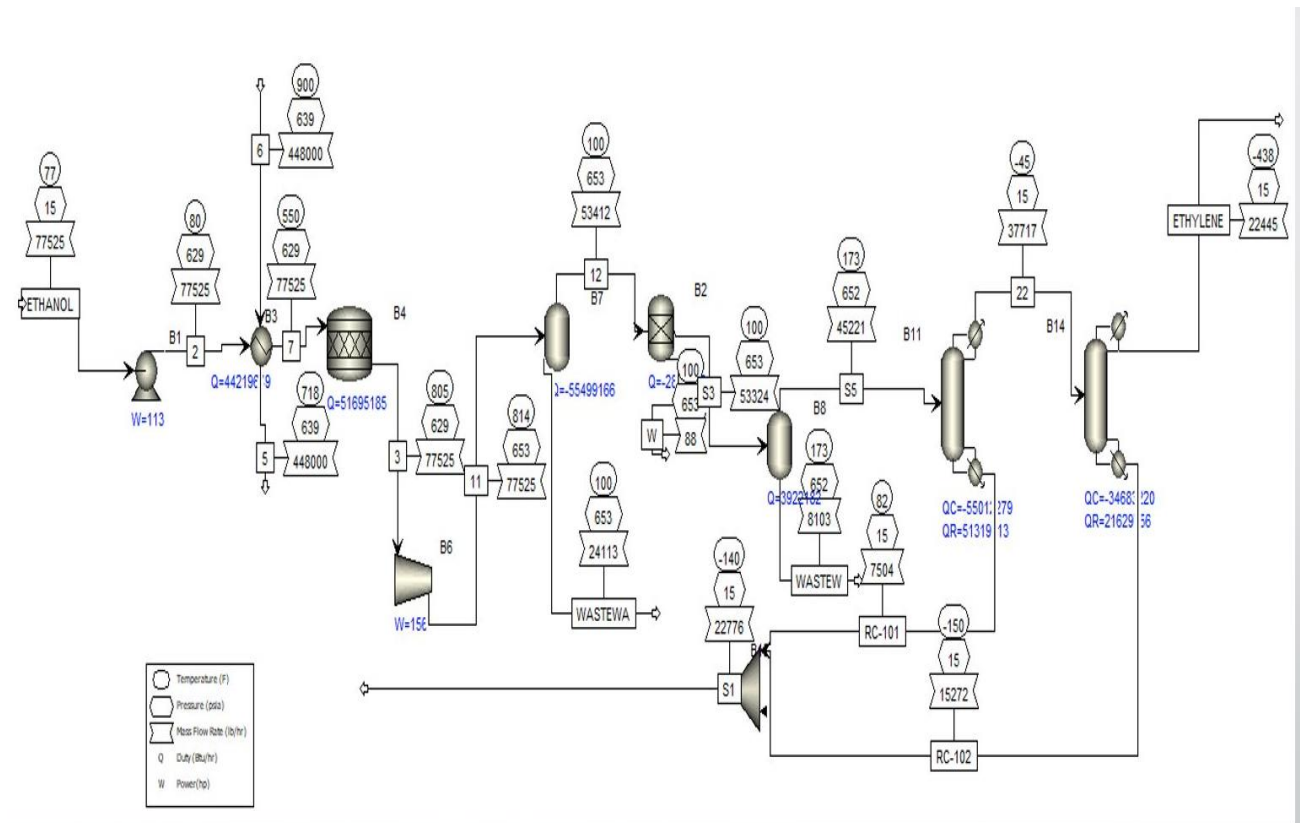


Figure 11: ASPEN / PLUS Model

8. Chemical Engineering Design

8.1 Design of Major Equipment

Along with the algorithm for the material balance of R-101 shown in 6.1.2. *Material Balance of major and supporting equipment*, we have the following algorithm used to derive the volume of the reactors.

$$1) V_{PBR} = \frac{W_c}{\rho_b}$$

$$W_c = 4197 \text{ kg / literature} \rightarrow 9252.80 \text{ lbs For } 69000 \text{ tons}$$

Now to upscale the catalyst weight

$$UPSC_{\text{Factor}} = \frac{400,000,000 \text{ lb/yr}}{120,000,000 \text{ lb/yr}} = 3.33$$

$$W_c (\text{catalyst weight}) = 9252.8 \text{ lbs} \cdot 3.33 = 30,811.82 \text{ lbs}$$

Now to use W_c to get V_{PBR}

$$V_{PBR} = \frac{W_c}{\rho_b} = \frac{30,811.82}{34 \text{ lbs/ft}^3} = 906.23 \text{ ft}^3 = 6709 \text{ gal}$$

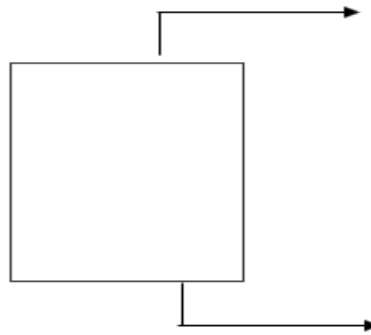
Knowing that our plant capacity would be 400,000,000 lb/hr, we were able to effectively determine the factor needed to upscale the amount of catalyst needed for our process in lbs. by comparing it to the plant capacity of the ethylene plant in Brazil that's producing 120,000,000 lbs/yr.

Once the upscale factor ($UPSC_{\text{Factor}}$) was identified, we applied it to the catalyst weight found in literature review and used the newfound catalyst weight to calculate the volume of R-101 given the catalyst bulk density of 34lbs/ft³. As a result, 6709 gal. was found to be the volume of the reactor.

-Reactor -101

Flash 101

Flash 101



Flow parameter

$$F_{lv} = \frac{W_l}{W_v} \sqrt{P_v / P_l}$$

Vapor Density

$$\begin{aligned} M_{wv} &= X(MW_{ethanol}) + MW_{ethylene} + MW_{water} \\ &= (.22)(46.07 \text{ g/mol}) + (.506)(20) + (.132)(2.37) \\ &= 20.5674 \end{aligned}$$

Volume of liquid

$$V_l = X(\text{H}_2\text{O})(18/0.9) + X(\text{C}_2\text{H}_4)(28.85/11.8)$$

Diameter

$$D = \sqrt{4(12)/3.14} = 4 \text{ ft}$$

Height

$$H_{total} = 3(3.76) = 12$$

$$0.77(10 \times 60) = 46.2 \text{ ft}$$

$$(77,525 \text{ lb/hr}) / 3600(68.046) = 1465.35$$

Pump-101

Pump Type

The type of pump used is a centrifugal pump.

Power Estimation

The constant volume and constant pressure specific heat values are obtained from ASPEN PLUS. The value of k is;

$$K = \frac{C_p}{C_v} = 1.101$$

Thus, value of “a” is as follows;

$$a = \frac{k - 1}{k} = \frac{1.101 - 1}{1.101} = 0.092$$

Thus, reversible adiabatic power is;

$$P = \frac{mzRT \left[\left(\frac{P_2}{P_1} \right)^a - 1 \right]}{a} = \frac{\left[\frac{4754}{3600} \right] 0.004331 (8.314) 298 \left[\left(\frac{624.7}{14.7} \right)^{0.092} - 1 \right]}{0.092}$$

$$P = 63.44 \text{ KW}$$

Pump Efficiency

The volumetric flow rate determined from Aspen is as follows.

$$V = 252.7 \frac{m^3}{h} = \frac{252.7}{3600} \frac{m^3}{s} = 0.07 \frac{m^3}{s}$$

For this volumetric flow rate, pump efficiency is 76%.

Exit Temperature

The exit temperature of the pump is determined from adiabatic compression:

$$T_2 = T_1 \left(\frac{P_2}{P_1} \right)^a = 298 \left(\frac{624.7}{14.7} \right)^{0.092} = 421K$$

8.2 Listing Equipment and Specification

P-101/102 Pump	HX-101/102 Heat Exchnager	R-101/102 Reactor	CM-101 Compressor	C-101/102 Cooler	FL-101/102 Flash Drum
AB-101 Absorber	DC-101 Distillation Column	CD-101/102 Condenser	CDC-101 Cryogenic Distillation Column	RC-101/102 Receiver	RF-101/102 Reflux Drum

Table 13: List of Equipment's

Ethanol and Water Reactor				
Identification:	Item:	Packed Bed Reactor (PBR) Alumina Catalyst		
	Item No:	R-101	Date	04/12/2022
	No. Required	1	By:	Group # 3
	C _{TPI} (\$)			\$89,500
Function:	To convert the reaction into the product			
Operation:	Continuous Batch Reactor (Agitated)			
	In	Out		
Materials Handled				
Mass Flow (lb/hr)	77525	77525		
Component Flow (Lb/Hr):				
Water	0	23646.6		
Ethylene	0	33990.4		
Ethanol	77525	3876.25		
Dimethyl-ether	0	7484.03		
Acetaldehyde	0	8154.29		
Hydrogen	0	373.156		
Temperature (F)	550	805		
Pressure (psig):	629	629		
Design Data:				
Material	Stainless Steel			
Volume	2072.14 ft ³			
Partial Size	(.01-.02) inches			
Catalyst Weight	9252.8 lbs			
Catalyst Bed Volume (gallons)	2035.75			

Table 14: Reactor 101 Specification Sheet

Ethanol – Water Pump				
Identification:	Item:	Centrifugal pump		
	Item No:	P-101	Date	04/12/2022
	No. Required	1	By:	Group # 3
	C _{TPI} (\$)	\$97,432		
Function:	To pump water and ethanol feedstock			
Operation:	Continuous			
	Product			
Materials Handled				
Total Flow(lb/hr):	77525			
Volumetric Flow(cuft/hr)	1558.63			
Component Flow (Kmol/hr):				
Water	0			
Ethylene	0			
Ethanol	77525			
Acetaldehyde	0.0			
Dimethyl-ether	0.0			
Hydrogen	0.0			
Temperature (F)	80			
Pressure (psig):	629			
Vapor Fraction:	0.0			
Design Data:				
Fluid Head(m)	531.39	Material:	Carbon Steel	
Efficiency (%)	76	Power (KW)	63.44	

Table 15: Pump 101 Specification Sheet

9. Economic Evaluation

To properly perform the economic analysis the basis of the equipment cost was a major contributor to the plant production. Each equipment price is based on the size needed to carry out the process. Through those calculations the capacity of the plant can be determined. Many factors were considered throughout the analysis to give an accurate cost estimate. Factors including cost of raw materials, utilities, taxes, insurance, and labor costs.

Summary of Economics			
Total Capital Investment (TCI)	Invested Capital	Total Operating Assets- Total Operating Liabilities + Total Non-Current Assets	31.89 million dollars
Net Present Value (NPV)	Difference between the current or expected future cash flows at various times.	$NPV = \frac{\sum R_t}{(1+i)^t}$	22.23 million dollars
Return on Investment	View of profitability of the plant after tax earnings the third year of operation if they remain unchanged during the project.	$ROI = \frac{(S - C)(1 - t)}{C_{tci}}$	32.6% per year
Discounted Rate of Return on Investment (IRR)	Time required for annual earnings to equal the original Investment.	$PBP = \frac{C_{tci}}{(1 - t)(S - C) + D}$	14.1% per year
Net Return	Internal rate of return after fees and carried interest are factored in.	$NPV = \sum_{n=0}^N \frac{C_n}{(1 - r)^n}$	4.2 million
Pay Back Period	Amount of time for the investment to recover our initial payout in terms of profits and savings.	Initial investment/ Cash Flow per year	2.1 years

Table 16: Summary of economics

The cash flow diagram shows the income and expenses over a 15-year period. Our initial investment at year one is the amount that is put into making our plant. After that investment you can see a slight increase in our revenue and have had a steady positive amount of cash flow through 15 years. This Ethelyne plant is a successful investment that an investor can make once all parts of the production are reviewed.

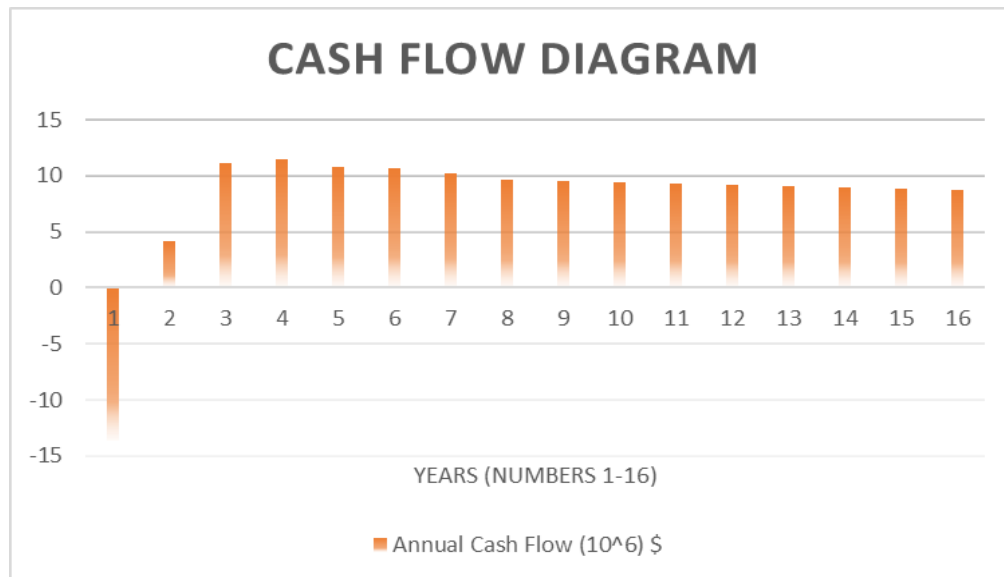


Figure 12: Cash Flow Diagram

10. Safety and HAZOP Analysis

We have performed our HAZOP Analysis over one of the major units in the plant. Our team decided to do a HAZOP Analysis over Reactor section in the PFD. We have Created a (P&ID) Piping and Instrumentation Diagram to help us effectively perform the HAZOP Analysis.

Ethanol is fed into the reactor at a pressure of 629 psig and temperature of 805°F. A temperature transmitter, pressure transmitter is being used throughout the reactor. The temperature sensor TT-12 will sense temperature and will transmit the signal to controller TIC-100 which will compare the signal with set point (operating temperature of reactor). Based on the error, an output signal will be sent to the feed valve which will adjust its flow rate so that temperature of reactor is set point. The pressure sensor PT-10 will sense pressure and will transmit the signal to controller PIC-100 which will compare the signal with set point (operating pressure of reactor). Based on the error, an output signal will be sent to the product valve which will adjust its opening so that pressure of reactor is set point. Finally, the product will come out at a 629°F pressure of 805 psig.

The image shows a very faint, low-contrast P&ID diagram of Reactor 101. It appears to be a horizontal rectangular vessel with various piping connections, valves, and instrumentation symbols (like circles with letters) distributed around it. The details are too light to discern clearly.

Figure 13: Reactor 101 P&ID

Hazard and Operability Analysis (HAZOP) – Reactor Stage

Process Unit: R-101 Reactor

Intention: The dehydration of ethanol to produce ethylene

The reactor is the most crucial stage in the process stream since it is responsible for the removal of water from preheated ethanol to produce ethylene and water. This reaction is illustrated as follows.

The project involves the development of an ethylene manufacturing plant in North Dakota, USA, and as such, the safety and precautionary measures under consideration should be in conformance with those of the state. North Dakota applies safety and management standards that are in line with those stipulated by the federal government through the Occupational Safety and Health Administration (OSHA). The relevant safety guidelines with regard to the establishment of a chemical plant for the purpose of synthesizing ethylene from ethanol in North Dakota are therefore as follows.

1910.119 Process Safety Management of Highly Hazardous Chemicals (Herman & Jeffress | OSHA, 2000)

Employee Participation: Employers shall:

- Consult with employees and their representatives on the conduct and development of process hazard analyses and development of other elements of process safety management. (1910.119.c.2)
- Provide employees with access to process hazard analyses (1910.119.c.3)
- Complete a compilation of written process safety information before conducting any process hazard analysis (1910.119.d)
- Document that equipment complies with recognized and generally accepted good engineering practices (1910.119. 3)
- Perform an initial process hazard analysis on processes covered.
- Use one or more of the following methodologies that are appropriate to determine and evaluate the hazards of the process being analyzed (Herman & Jeffress | OSHA, 2000):
 - i) What-if;
 - ii) Checklist.
 - iii) What-if/checklist.
 - iv) Hazard and Operability Study (HAZOP).
 - v) Failure Mode and Effects Analysis (FMEA).
 - vi) Fault Tree Analysis; or
 - vii) An appropriate equivalent methodology.

A hazard and operability (HAZOP) analysis presents a means of determining and documenting how the reactor's deviation from its design intent can create risk for personnel and equipment, the possible consequences and how this deviation can be mitigated to uphold safety.

To conduct a HAZOP analysis an examination of all the streams leading to and from the reactor as well as the materials and conditions associated with the prescribed reaction is necessary. In this regard, the feed stream to the reactor contains ethanol which is fed to reactor at a pressure of 629 psi and a temperature of 805 °F. On the other hand, there is a single product stream leaving the reactor containing a mixture of ethylene and water. This line is also at a pressure of 629 psig and a temperature of 805 °F. The reactor itself contains a γ -alumina catalyst which facilitates the dehydration process. This information is summarized as follows:

	Feed stream (ethanol)	Product stream (ethylene + water mixture)
Temperature	805 °F	805 °F
Pressure	629 psig	629 psig
Catalyst	γ - alumina catalyst	

Table17: Reactor-101 Conditions

Because both ethanol and ethylene are highly flammable substances, the HAZOP analysis must account for measures to regulate both temperature and pressure within the reactor. There are also other relevant risks that can be addressed to ensure that operations within the reactor are conducted in a safe manner. The following HAZOP analyses shed light on some of these risks and mitigative measures that should be put in place.

I. R-101 Feed Line – Entry of reactant (ethanol) into the reactor.

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Flow	None	No flow to R-101	There is no flow of ethanol into the reactor	- Feed line valve is closed. - Blockage in the feed line	-No reactant enters the reactor	-Alarm /monitoring system at the feed line valve	- Opening the feed line valve. - The installation of a bypass system in case of blockages
		More	More flow into R-101	There is an increase of ethanol flow into the reactor	- Control valve failure. - Failure of operator to take action on alarm	-Inefficiency of the reactor because of failed	- Installation of a metering system at the control valve	- Following the stipulated maintenance schedule and

						catalytic conversion	to regulate and measure flow.	procedures by operator
2	Temperature	More	Increase in feed temperature	There is sudden increase in temperature at the feed of R-101	- Incorrectly calibrated temperature gauge	- Thermal runaway and risk of explosion. Ineffectiveness of the catalyst	- Temperature alarm at feed entry point. - Recalibration of temperature gauge	- Installation of a temp gauge - Checking maintenance schedule and procedures
3	Pressure	More	Pressure build-up in the feed line	There is pressure building up in the feed line leading into the reactor	- Clogging /Blockage in the line. - Failed reaction in the reactor	- Failure of feed line tube - Risk of expansion and bursting of the reactor	- Installation of quick-pressure relief valves at strategic locations before and after the reactor.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure loss in feed line	There is pressure loss in the feed line to the reactor	- Faulty pump (P-101). - Inadequate or low levels of ethanol in the tank	- Insufficient reactant material entering the reactor	- Pressure gauge at the pump and in the feed line	- Installation of pressure gauge - Checking and adhering to the maintenance schedule and procedures

Table18: Feed Line HAZOP

II. Within the Reactor (R-101) – Alumina Catalyst ($\gamma\text{-Al}_2\text{O}_3$) Facilitates the Dehydration of Ethanol

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increases in the reactor	There is pressure build up in the reactor	- Blockage further in one of the product lines. - Incomplete reaction in the reactor. - Increased flow from the feed line - Failure of operator to take action on alarm.	- Risk of expansion, bursting and/or damage to the reactor. - Inefficiency of the Alumina catalyst	- Installation of quick-pressure relief valves at strategic locations within the product line	- Installation of a secondary pressure relief device. - Checking and following maintenance schedule and procedures
		Less	Pressure decreases in the reactor	There are sudden pressure losses in the reactor	- Leakages within the in the feed line. - Influx of flow rate in the product lines	- Less reactant is converted to product - Inefficiencies	- Pressure monitoring devices before and after the reactor	- Installation of pressure gauge - Checking and following

						within the reactor		maintenance schedule and procedures
2	Temperature	More	Temperature increases in the reactor	There is a sudden increase in temperature within the reactor	-Failure of reactor cooling devices	-Deactivation of the Alumina catalyst. - Incomplete conversion of reactant to product	-Installation of a cooling jacket or other cooling techniques	-Installation of a temp gauge - Checking and following maintenance schedule and procedures

Table 19: Within the Reactor HAZOP

III. R-101 Product Line – Transportation of ethylene and water mixture from the first reactor (R-101) to the second reactor (R-102).

No	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Flow	Reverse	Back flow to R-101	There is a backflow of the product stream back to the reactor	- Pressure loss in the product line. - Clogging and blockage down the product line	-Mixing of reactant and product in the reactor. -Inefficiencies within the reactor	- Check valve to prevent back flow	-Monitoring pressure in the product line, -Following the stipulated maintenance schedule and procedures
		More	More flow in product line to the second reactor	There is an increase in the flow of product leaving the reactor.	- Control valve failure. - Incomplete reaction in the reactor - Failure of operator to take action on alarm	- Pressure build-up in the line. - Potential leakages and bursting of the product line.	- Installation of an alarm system to monitor the flow rate of product leaving the reactor.	- Following the stipulated maintenance schedule and procedures by operator
2	Temperature	More	Increase in product line temperature	There is a sudden increase in temperature within the product line.	- Incorrectly calibrated temperature gauge within the line. - Product buildup going into the second reactor	-Risk of thermal runaway. - Failure of product line including expansion and bursting.	- Recalibration of temperature gauge within the line. - Flow regulation throughout the product line	-Installation of a temp gauge - Checking and following maintenance schedule and procedures
3	Pressure	More	Pressure increases in the	There is pressure build up in	-Blockage further up the product	- Failure of the product line tube	-Installation of quick-pressure	- Installation of a secondary

			product line	the product line transporting ethylene and water from the reactor	line or in the second reactor. -Incomplete reaction in the first reactor. - Failure of operator to take action on alarm.	- Risk of expansion, bursting and/or damage to the downstream	relief valves at strategic locations within the product line	pressure relief device. - Checking and following maintenance schedule and procedures
		Less	Pressure decreases in product line	There are sudden pressure losses in the product line from the first reactor	- Clogging in the first reactor. - Leakages within the product line	- Less ethylene delivered to the mixer. - Backflow into the reactor	-Pressure monitoring devices within the product line	- Installation of pressure gauge - Checking and following maintenance schedule and procedures

Table20: Product Line HAZOP

11. Discussion

Throughout the course of this project, we have made many assumptions based on literature reviews. Our temperatures and pressures were referenced from basic knowledge of the chemicals and their boiling and melting points. Thus, multiple values were obtained. Our material balance and energy streams are as accurate as we could get them to run our process on ASPEN PLUS.

12. Conclusions and recommendations

For the first half of our project, we were successfully able to create a design from scratch that produces ethylene from ethanol. We went through an incredibly detailed process analysis and economic analysis to give us the best feasible options for our design. Much research was done to complete such a task including Process flow diagram, Material Balances, and the types of equipment that is needed for our plant.

13. Refence References

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15. Herman, A., & Jeffress, C. (2000). *Process Safety Management* [Ebook]. Occupational Safety and Health Administration. Retrieved 15 April 2022, from <https://www.osha.gov/sites/default/files/publications/osha3132.pdf>.
- 16.

14. Appendix

14.1 Sample calculations

14.1.1 One example clearly explaining each type of calculation should be presented

14.1.2 Computer simulations used

We have used Visio to create the Block Flow Diagram and Process Flow Diagram. Aspen Plus was used for the simulations.

14.1.3 Derivation of essential equations that enable an understanding of report not presented in detail in the main body of the report

14.2 Tables of data used with reference to sources

**SENIOR DESIGN AND PROFESSIONALISM II
SPRING 2022**

Title of Assignment: Final Project Powerpoint Presentation

The grading rubrics for evaluation of the Senior Design II projects CHEG 4248 (a continuation of the fall 2021 Senior Design I CHEG 42472) are presented below. The students are to be evaluated as outlined in the rubrics with emphasis on the following:

- Justification of plant location and capacity
- Provide a process description and Process Flow Diagram (PFD) for the plant showing the major items of equipment, and indicating the materials of construction and the operating temperatures and pressures
- Material and energy balances with summary table for the process with streams information showing a mass balance for each major equipment
- A complete HYSYS/ASPEN simulation report of the process
- Chemical engineering design of major equipment such as (i) reactor(s), (ii) absorption column(s) and (iii) distillation columns
- Estimates of the Major Equipment Capital Cost (Capex)
- Estimates of Operating Cost (Opex)
- Preparation of a net present value and investor's rate of return analysis for the investment over a 15-year life, assuming the company's current capital hurdle rate is 15%.
- Preparation of a project milestone schedule
- Preparation of a P&ID for a section of the process showing the control scheme to ensure safe operation of the unit, and carrying out a HAZOP analysis of the section of the process selected
- Preparation of a safety report indicating the safety measures required for the plant bearing in mind any toxic and flammable materials handled

In addition, the names of the presenters for each design project have been included in the rubrics to enable each presenter to be evaluated as well.

References:

- 1. Gael D. Ulrich and Palligarnai T. Vasudevan, "Chemical Engineering : Process Design and Economics, A practical Guide", second edition, 2004, Process Publishing, New Hampshire, USA, ISBN 0-9708768-2-3**
 - 2. Gavin Towler and Ray Innott, "Chemical Engineering Design : Principles, Practice and Economics of Plant and Process Design" Butterworth-Heinemann, ISBN 978-0-08-096659-5, second edition, 2013**
 - 3. Perry's Chemical Engineering Handbook, sixth edition or latest**
-
- 4. Turton, R., Bailie, R., Whiting, W., and Shaeiwits, J. A. "Analysis, Synthesis, and Design of Chemical Processes," 4th Edition Prentice-Hall PTR, Upper Saddle River, New Jersey 07458, 2008.**
 - 5. "Plant Design and Economics for Chemical Engineers" by Peters, M.S., K.D. Timmerhaus and R.E. West, 5th edition, 2003, McGraw-Hill, ISBN 0-07-239266-5.**

**DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM II CHEG 4248
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR SPRING 2022 SEMESTER**

ABET Student Learning Outcome 3: An ability to communicate effectively with a range of audiences (Written Technical Communication)

Assignments that test competency in written communication will include problems that test the student's ability to logically arrange information, use correct grammar, use appropriate format, use discipline specific conventions including citations, and use acceptable graphical conventions.

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Points Assigned	Points Received
1. Ability to prepare an executive summary for the report	10	
Students are able to prepare an executive summary of 5 to 8 pages	10	
2. Ability to organize, plan and properly format a written technical report	80	
(i) Students are able to organize report by categorizing ideas for the report into well and logically organized chapters, major sections, subsections and paragraphs blended within the larger units.	20	
(i) Students are able to organize report by categorizing ideas for the report into well and logically organized chapters, major sections, subsections and paragraphs blended within the larger units.	20	
(ii) Students provide Title Page, and Table of Contents, list of Figures, and List of Tables properly formatted.	12	
(iii) Students provide figure number and title for each figure in the report, reference each figure, and completely discuss each figure in the report in accord with standards in the project manual.	12	
(iv) Students provide table number and title for each table in the report in accord with standards in the project manual, reference each table, and completely discuss each table in the report.	12	
(v) Students properly cite references in the report and provide well formatted reference list at the end.	12	
(vi) Students prepare the written report in accord with standard report formatting provided in the Senior Projects Report Manual.	12	
3. Ability to compose original texts and properly apply the conventions of written language	50	
(i) Properly apply capitalization, punctuation, and penmanship, to communicate clearly.	15	
(ii) Spell proficiently	10	
(iii) Apply standard grammar and usage to communicate clearly and effectively in writing including • using complete sentences, varying the types such as compound and complex to match meanings and purposes • properly employing standard English usage in writing for audiences, including subject-verb agreement, pronoun referents, and parts of speech • properly using adjectives (comparative and superlative forms) and adverbs appropriately to make writing vivid or precise • properly using prepositional phrases to elaborate written ideas • properly using conjunctions to connect ideas meaningfully	20	
(vi) Use available technology to support aspects of creating, revising, editing, spell checking, and publishing the report.	5	
4. Ability to provide appropriate discussion, conclusions and recommendations	60	
(i) Summarize the goals, objectives, and indicate whether they were met.	10	
(ii) Summarize the results.	30	
(iii) Summarize constraints and codes and indicate whether they were met.	10	
(iv) Provide logical conclusions and recommendations (including strengths and weaknesses).	10	
Total	200	

SENIOR DESIGN & PROFESSIONALISM II CHEG 4248

Oral Design Presentation Evaluation Form

Title of Presentation:

Date of Presentation: April 23, 2022

Name of Examiner/Appraiser:

Performance Criteria	Not Acceptable (0-59.9%)	Below Expectations (60-69.9%)	Average meets minimal expectations 70-79.9	Very Good Meets Expectations (80-89.9%)	Excellent Exceeds Expectations (90-100%)
1. Ability to Organize, Plan, Design/Prepare and Use Appropriate Visual Aids for communication/Presentation**	20 40 59	60 65 69	70 75 79	80 85 89	90 95 99
Presentation is organized in well structured logical sequence making it easy for audience to follow the content with clear understanding.	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Slides are well prepared and are effective in helping audience to understand (<i>adequate and relevant technical content and view graphs that are legible, completely labeled, annotated, dimensioned to illustrate important features of the work being presented</i>)	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Modern presentation techniques are used (<i>may include visually enhanced transitions, animations, video, and sound clips</i>).	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Average for this Performance Criteria					
2. Ability to Articulate Subject Knowledge (Technical Content)*					
Client identification and recognition of need	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Project goals and objectives, and planning	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Process screening and selection, PFD and process description	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Process chemistry, and material and energy balances	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Quality of chemical engineering design/and analysis, and design constraints	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Design within economic, societal and environmental constraints(including contemporary issues and broader impact on society)	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Hazard and Safety considerations*****	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Questions are responded to in a clear professional manner after restating questions to audience	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Average for this Performance Criteria					
3. Appearance and Ability to Provide Good Oral Delivery**					
Correct grammatical English and technical terms appropriate to technical area and audience are used; and presenters speak with clarity and confidence	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Good posture and eye contact with the audience are maintained (<i>should not read from prepared notes</i>) and elicits the attention of the audience	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Presenters dress appropriately for the occasion.	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Efforts of all group members/Group dynamics***	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Average for this Performance Criteria					
OVERALL AVERAGE GROUP PERFORMANCE					
NAME OF PRESENTER	OVERALL PERFORMANCE OF PRESENTER				
	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
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	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
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*ABET Student Outcome 2 ; **ABET Student Outcome 3; *** ABET Student Outcome 5; ****Program Criterion 9b

ABOVE AVERAGE

**Above Average Student Original Graded Assignment on Final Project
Powerpoint Presentation**

PRODUCTION OF DIMETHYL ETHER

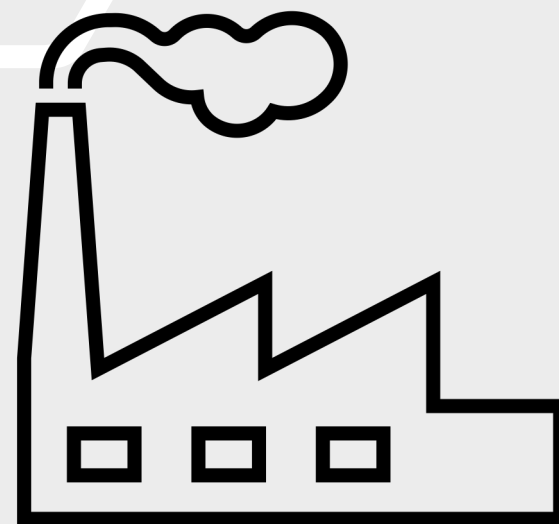
DADA TEAM 4

Amiya Rogers — 88%

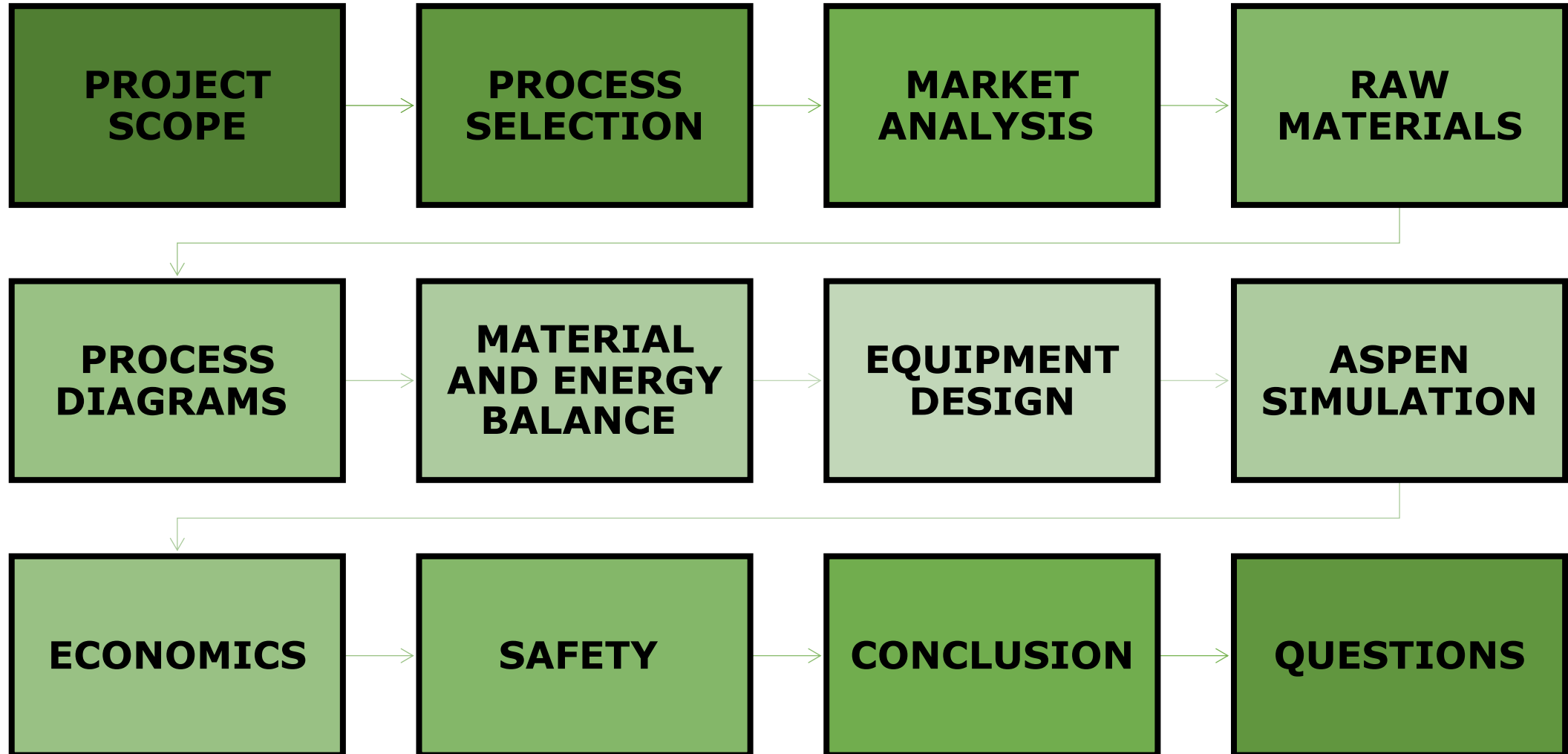
Cinthia Sahin — 88%

Laura Ukpede — 87%

Taylon Owens — 90%



OUTLINE



PROJECT SCOPE

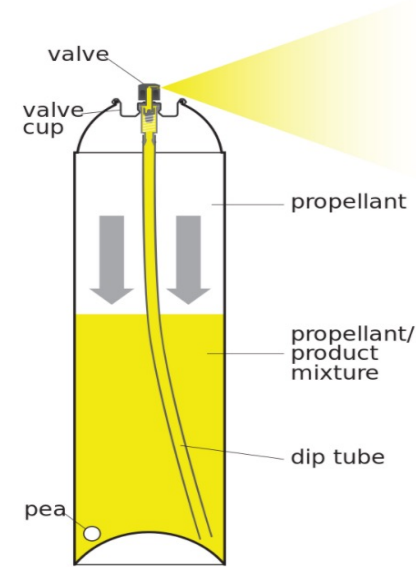
PROBLEM STATEMENT

The purpose of this project is to design a system that produces Dimethyl Ether (DME) at the required 99.9% purity.



PRODUCT USES

- Refrigerant (R-E170)
- Solvent
- Propellant in industrial aerosol products.
- Potential use for transportation fuel, domestic use, and power generation



PROCESS SELECTION

PROCESSES CONSIDERED

ALTERNATIVE	PROCESS	PROS	CONS
1	Methanol Dehydration	- Consumes less time and cost of equipment - Relatively simpler process flow - Catalyst deactivation occurs at relatively high temperature (400 C).	- Requires more downstream separation technologies. - Sourcing of methanol may present challenges. - Marginally lower DME yield.
2	Indirect Synthesis from biogas feedstock	- Marginally higher DME yield. - Water build up in the process is alleviated. - Energy efficiency is maximized.	- Sourcing of biogas feedstocks presents a challenge. - Process requires more equipment. - Relatively costly and time consuming
3	Direct Synthesis from Natural Gas Feed Stock	- Higher Yield of DME. - Low production cost. - Abundantly available feedstock	- Highly exothermic. - Low production rate - Higher operating temperature.

PROCESS SELECTION MATRIX

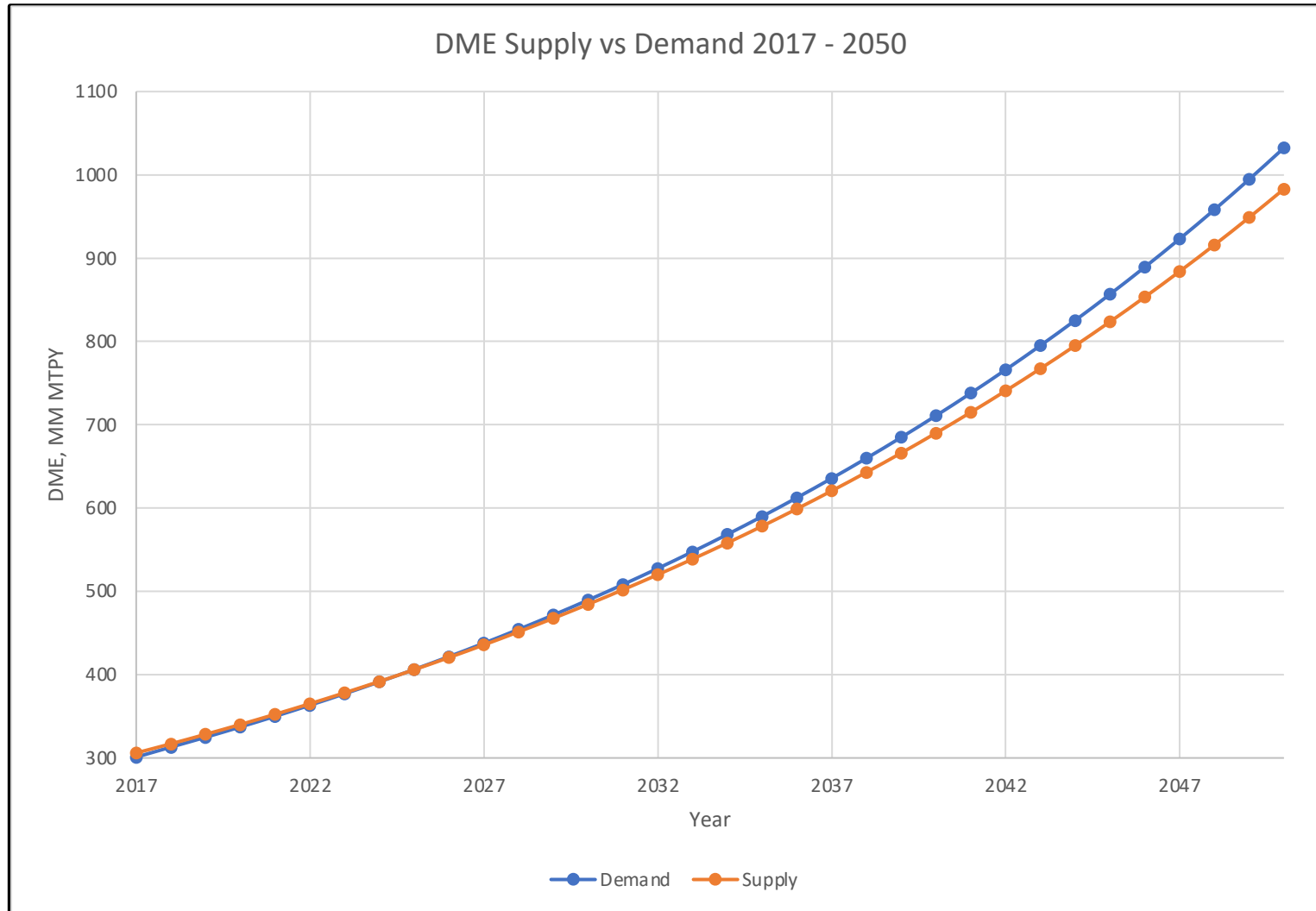
CONSIDERATIONS	ALTERNATIVE 1 Methanol Dehydration	ALTERNATIVE 2 Indirect Synthesis from biogas feedstock	ALTERNATIVE 3 Direct Synthesis from Natural Gas Feed Stock	WEIGHT
Economics	18	10	12	40%
Environmental	13	16	20	25%
Location	14	13	9	25%
Safety	13	13	16	10%
Total	<u>15.25</u>	12.5	13.65	100%

PROJECT PLANNING (GANTT CHART)

PROJECT TITLE:		PRODUCTION OF DIMETHYL ETHER (DME)																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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MARKET ANALYSIS

MARKET ANALYSIS



PLANT STARTUP:

2026

2 Year Build-Time

DEMAND BASIS:

50,000 Metric Tons Per Year
(5% of 1MM Gap)

DEMAND BASIS:

90% Utilization

CLIENT IDENTIFICATION



PLANT LOCATION

LOCATION:

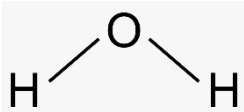
Plaquemine, Louisiana

Plaquemine Cogeneration Facility: Steam and Power
Port of Plaquemines for Cooling Water



RAW MATERIALS

CHEMICAL CONDITIONS

Conditions	Methanol	Dimethyl Ether	Water
Molecular Weight	0.071 lb/mol	0.102 lb/mol	0.039 lb/mol
Chemical Formula	CH ₃ OH	CH ₃ OCH ₃	H ₂ O
Chemical Structure	$ \begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{O}-\text{H} \\ \\ \text{H} \end{array} $	$ \begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{O}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array} $	
Boiling Point	148.46 ° F	-11.2°F	212°F
Melting Point	-138.28°F	-221.8°F	32°F
Flash Point	49.46°F	-41.98°F	-
Density	0.029 lb/in ³	0.071 lb/in ³	0.036 lb/in ³

RAW MATERIALS



A (Methanol)

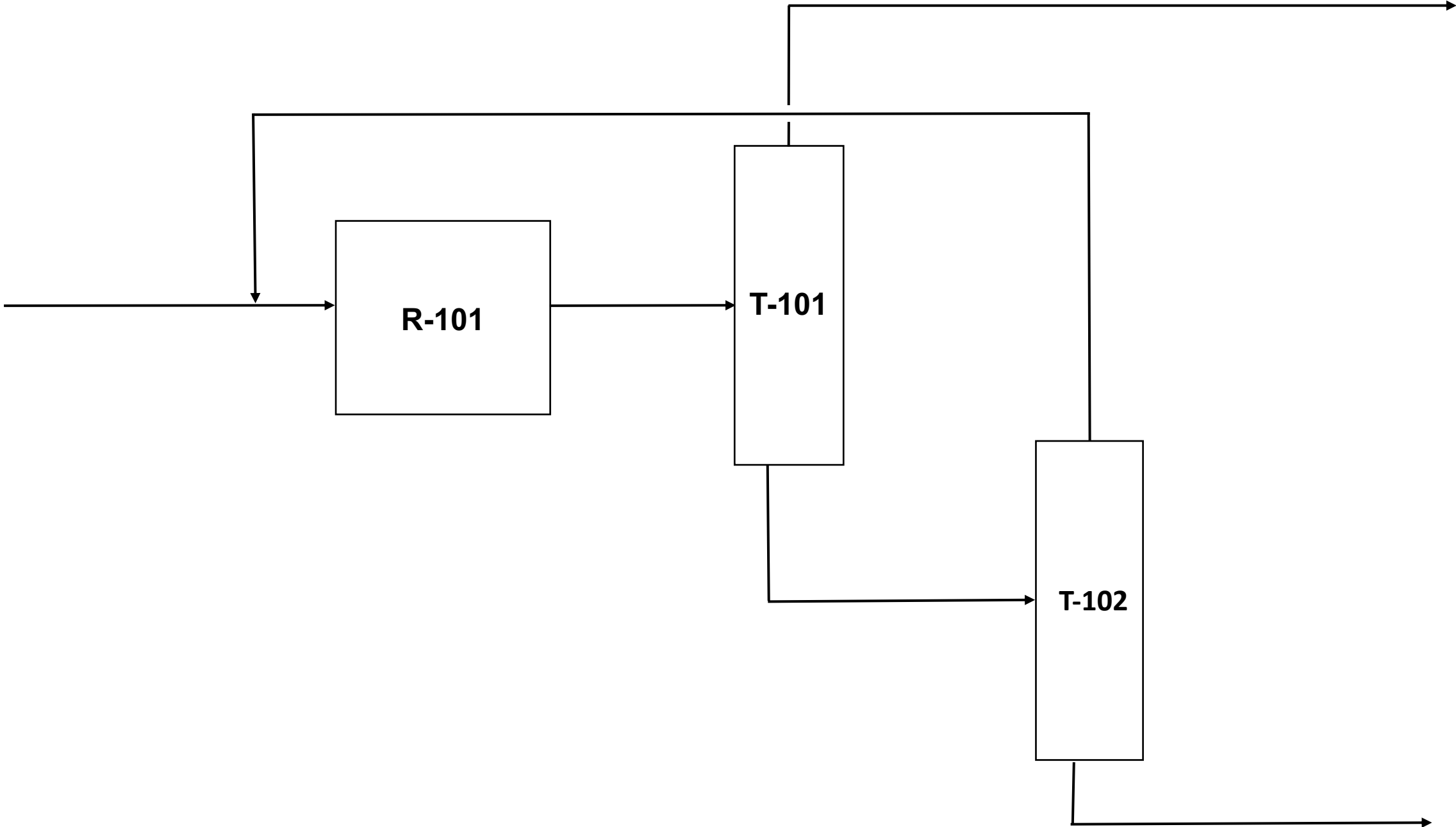
B (DME)

C (Water)

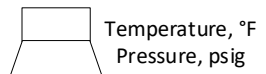
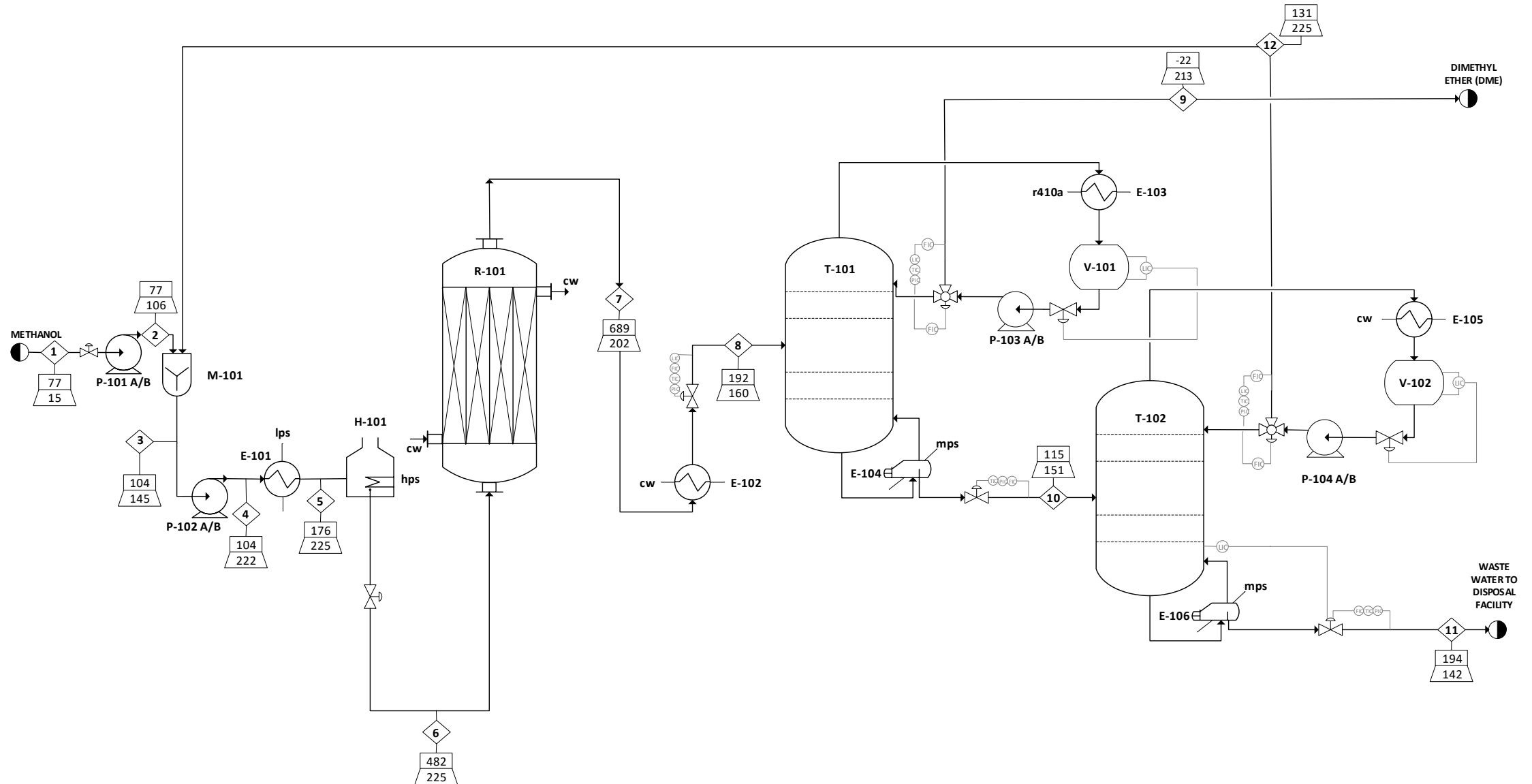
	A	B	C
mol	2	1	1
Molecular Weight lb/mol	0.071lb/mol	0.102 lb/mol	0.040 lb/mol
lb	0.141 lb	0.102 lb	0.040 lb
lb/lb DME	3.06 lb	2.20 lb	.862 lb
cents/lb	\$0.16	\$0.41	\$0.24

PROCESS DIAGRAMS

BLOCK FLOW DIAGRAM

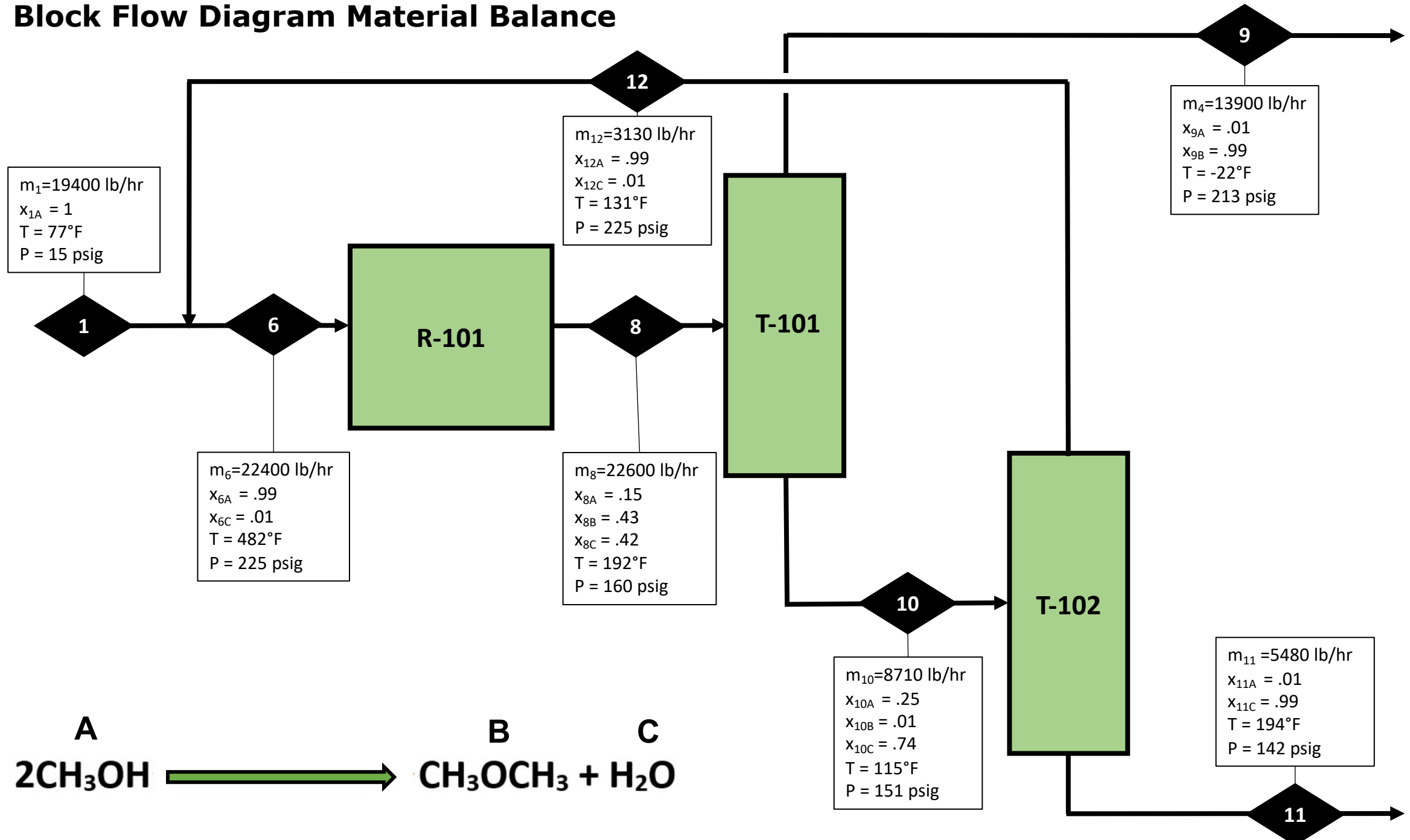


PROCESS FLOW DIAGRAM



MATERIAL AND ENERGY BALANCE

Block Flow Diagram Material Balance



MATERIAL BALANCE

STREAM CONDITIONS

Stream Description	Pure Methanol to Pump	Pure Methanol to Mixer	Mixed Stream to P-102	Methanol to Vaporizer	Combined Methanol to Furnace	Combined Feed to R-101	Reactor Effluent to Cooler	Methanol+ DME + Water to T-101	Dimethyl Ether Product	Methanol + Water to T-102	Wastewater to Disposal	Recycled Methanol to Mixer
Steam Number	1	2	3	4	5	6	7	8	9	10	11	12
Temperature (F)	77	77	104	104	176	482	689	192	-22	115	194	131
Pressure (psig)	15	106	145	222	225	225	202	160	213	151	142	225
Methanol Mole Fraction	1	1	.99	.99	.99	.99	.15	.15	.01	.25	.01	.99
DME Mass Fraction	0	0	0	0	0	0	.43	.43	.99	.01	0	0
Water Mass Fraction	0	0	.01	.01	.01	.01	.42	.42	0	.74	.99	.01
Mass Flow (lb/hr)	19352	19352	Methanol 22268	Methanol 22268	Methanol 22268	Methanol 22268	Methanol 3374	Methanol 3374	Methanol 97	Methanol 3203	Methanol 97	Methanol 3107
			Water 126	Water 126	Water 126		DME 13907	DME 13907	DME 13776	DME 184	Water 5382	
						Water 5307						Water 5307

ENERGY BALANCE

Methanol Dehydration R-101	
Temperature	689°F
R-101 Duty	-1.36×10^7 BTU/hr
E-101 Duty	9.67×10^6 BTU/hr
H-101 Duty	5.40×10^6 BTU/hr
E-102 Duty	-1.14×10^7 BTU/hr

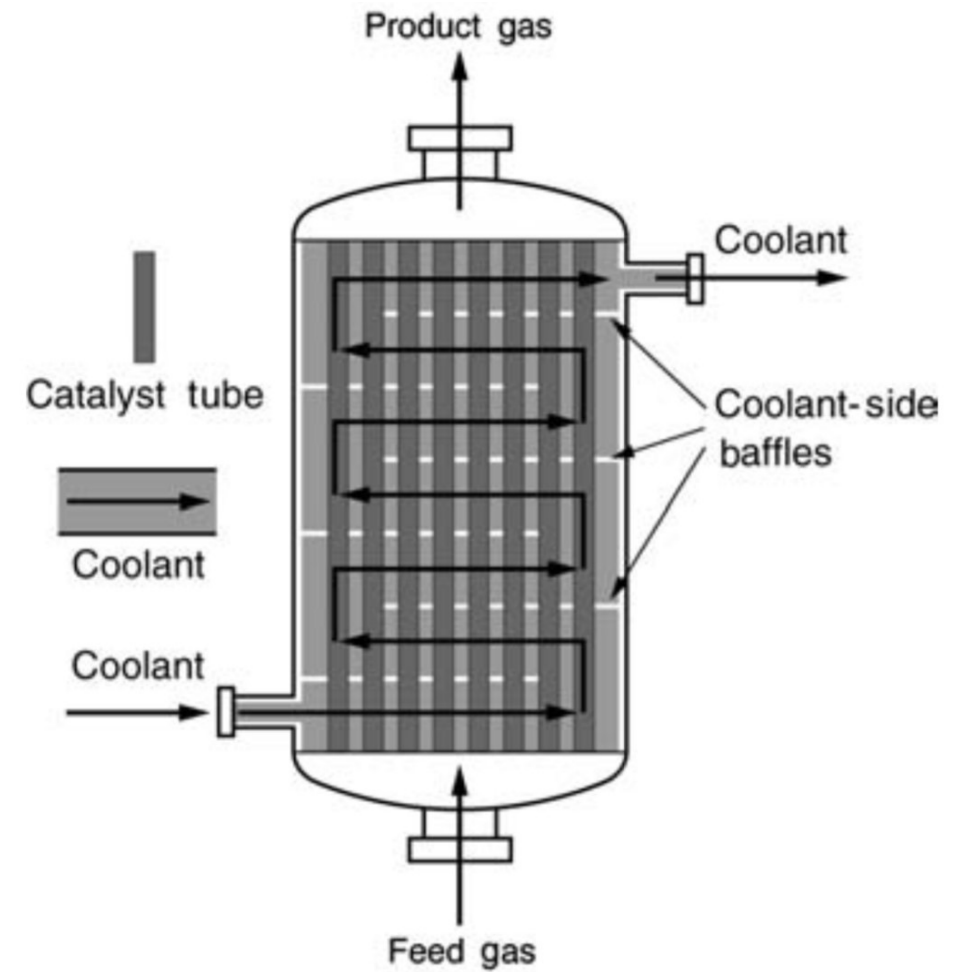
DME Distillation T-101	
Temperature	86°F/114.8°F
E-103 Duty	-3.39×10^6 BTU/hr
E-104 Duty	2.36×10^6 BTU/hr

Methanol Distillation T-102	
Temperature	158°F/194°F
E-105 Duty	-1.18×10^7 BTU/hr
E-106 Duty	1.14×10^7 BTU/hr

EQUIPMENT DESIGN

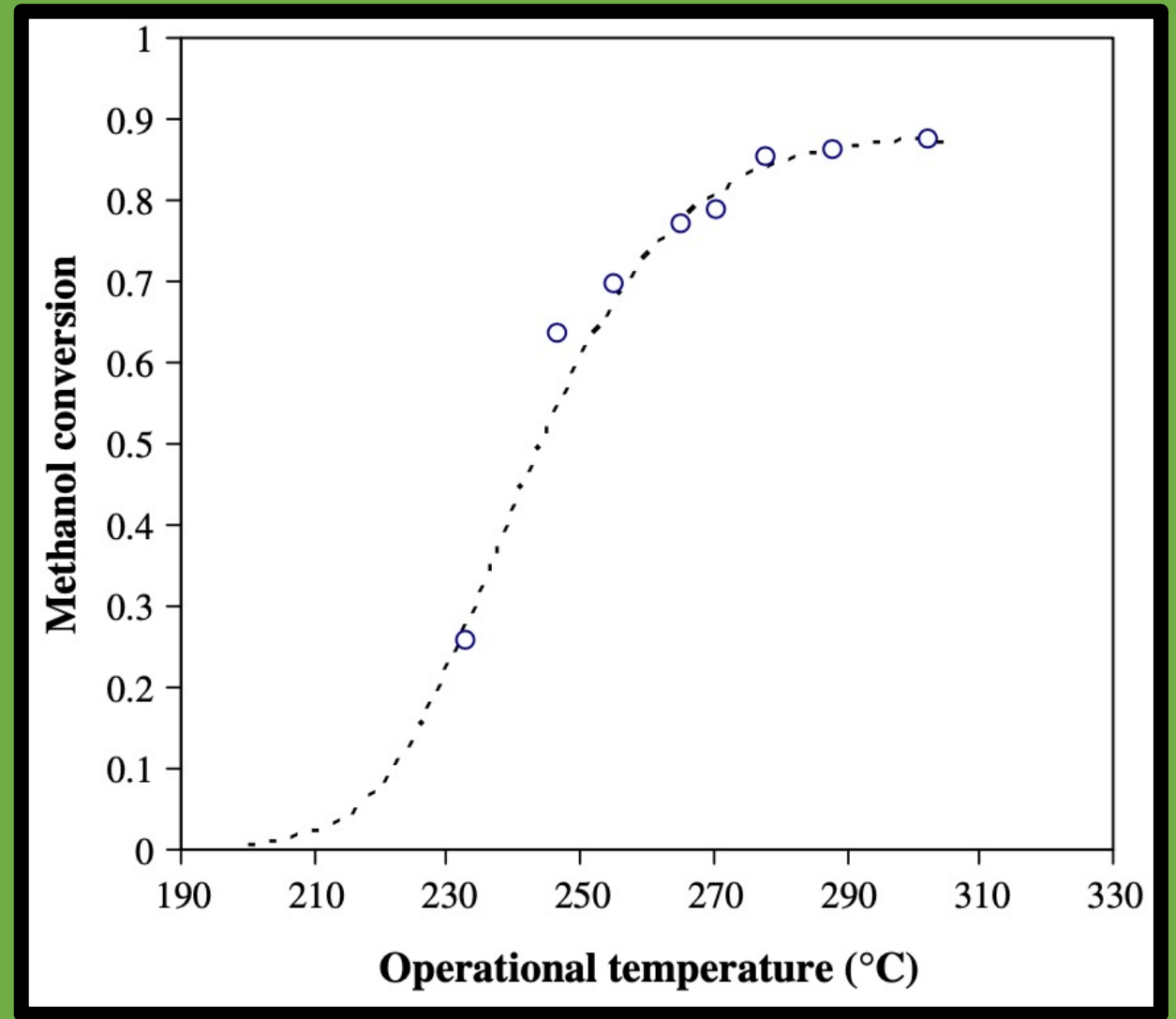
REACTION KINETICS

- Reaction: Methanol Dehydration
- Reactor Type: Catalytic Packed Bed Reactor
- Catalyst: $\gamma\text{-Al}_2\text{O}_3$
- Conversion: 90%
- Exothermic Reaction



CATALYST: γ -Al₂O₃

- Operates at high pressure
- Commonly used catalyst for Methanol Dehydration
- High activity
- Increase temperature ensures increased conversion



R-101 Specifications Sheet

Identification	
Item	Catalytic Packed Bed Reactor
Item No	R-101
Function	Dehydration of methanol to produce DME and water
Operation	Continuous
Catalyst	γ -Al ₂ O ₃
Catalyst Weight	54900 lbs

Materials Handled	In	Out
Mass Flow (lb/hr)	22400	22600
Mole flow (lbmol/hr)	702	702
Component Flow lbmol/hr		
Dimethyl Ether	0	302
Methanol	695	105
Water	7	295
Temperature (°F)	482	689
Pressure (psig)	225	202
Vapor Fraction	1.0	1.0

Design Data	
Diameter (ft)	4.36
Overall height (ft)	14.7
Number of Tubes	34
Maximum Pressure rating (psig)	218
Combined Tube Volume ft ³	62.3
Area (ft ²)	40.7
Construction of Material	Carbon Steel
Utilities (CW)	28600
Duty (Btu/hr)	-1.36x10 ⁷
Comments	-Temperature maintained by cooling water. - Shell side Methanol -Tube Side Water

T-101 Specifications Sheet

Identification	
Item	1 st distillation column
Item No	T-101
No. Required	1
Function	Separates DME from methanol and water
Operation	Continuous
Material Of Construction	Carbon Steel

Design Data	
Number of actual trays	22
Total tower height (ft)	52.5
Column diameter (ft)	2.62
Maximum Pressure rating (psig)	218
Reflux ratio	1.7
Tray Spacing (ft)	2.00

Materials Handled	Feed Methanol + DME + Water	Liquid Distillate Methanol + DME	Liquid Bottoms Methanol + Water
Mass Flow (lb/hr)	22600	13900	8710
Mole flow (lbmol/hr)	702	302	400
Component Flow lbmol/hr			
Dimethyl Ether	302	299	400
Methanol	105	3.02	100
Water	295	0.00	296
Temperature (°F)	192	86	115
Pressure (psig)	151	165	162
Vapor Fraction	1	1	0.0

Associated Components					
Condenser (E-103)	CW = 185000 lb/hr	A = 330 ft ²	Q = 3.21 x 10 ⁶ Btu/hr	- Fixed Head - Carbon Steel	Max Pressure = 145 psig
Reboiler (E-104)	mps = 2770 lb/hr	A = 72.2 ft ²	Q = 2.24.10 ⁵ Btu/hr	- Floating Head -Carbon Steel	Max Pressure = 160 psig
Reflux Drum (V-101)	L = 9.48 ft	D = 3.74 ft	Carbon Steel	Max Pressure = 149 psig	
Reflux Pump (P-102 A/B)	Power = 5.2 kW	Efficiency = 40 %	ΔP = 66.7 psig	Centrifugal/Carbon Steel	

T-102 Specifications Sheet

Identification	
Item	2 nd distillation column
Item No	T-102
No. Required	1
Function	Separates methanol from water
Operation	Continuous
Materials Of Construction	Carbon Steel

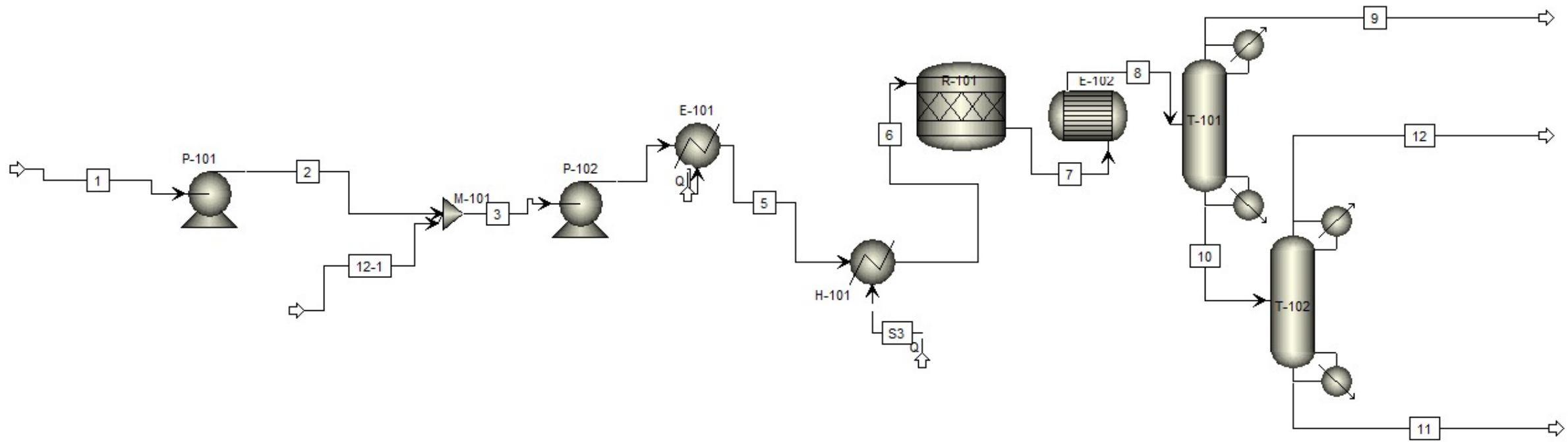
Design Data	
Number of actual trays	15
Total tower height (ft)	65.6
Column diameter (ft)	3.81
Maximum Pressure rating (psig)	218
Reflux ratio	4.5
Tray Spacing (ft)	2.62

Materials Handled	Feed	Liquid Distillate	Liquid Bottoms
Mass Flow (lb/hr)	8710	3120	5480
Mole flow (lbmol/hr)	400	98	302
Component Flow lbmol/hr			
Dimethyl Ether	3.99	0.00	0.00
Methanol	100	97	3.02
Water	29	0.970	299
Temperature (°F)	114	158	194
Pressure (psig)	162	106	107
Vapor Fraction	0.0	1.0	0.0

Associated Components					
Condenser (E-105)	CW = 649000 lb/hr	A = 74.45ft ²	Q = 1.18x10 ⁷ Btu/hr	- Fixed Head - Carbon Steel	Max Pressure = 102 psig
Reboiler (E-106)	mps = 100 lb/hr	A = 272 ft ²	Q = 1.14x10 ⁷ Btu/hr	- Floating Head - Carbon Steel	Max Pressure = 160 psig
Reflux Drum (V-102)	L = 8.30 ft	D = 12.3 ft	Carbon Steel	Max Pressure = 2160 psig	
Reflux Pump (P-103 A/B)	Power = 1.0 kW	Efficiency = 40 %	ΔP = 55.5 psig	Centrifugal/Carbon Steel	

ASPEN SIMULATION

SIMULATION

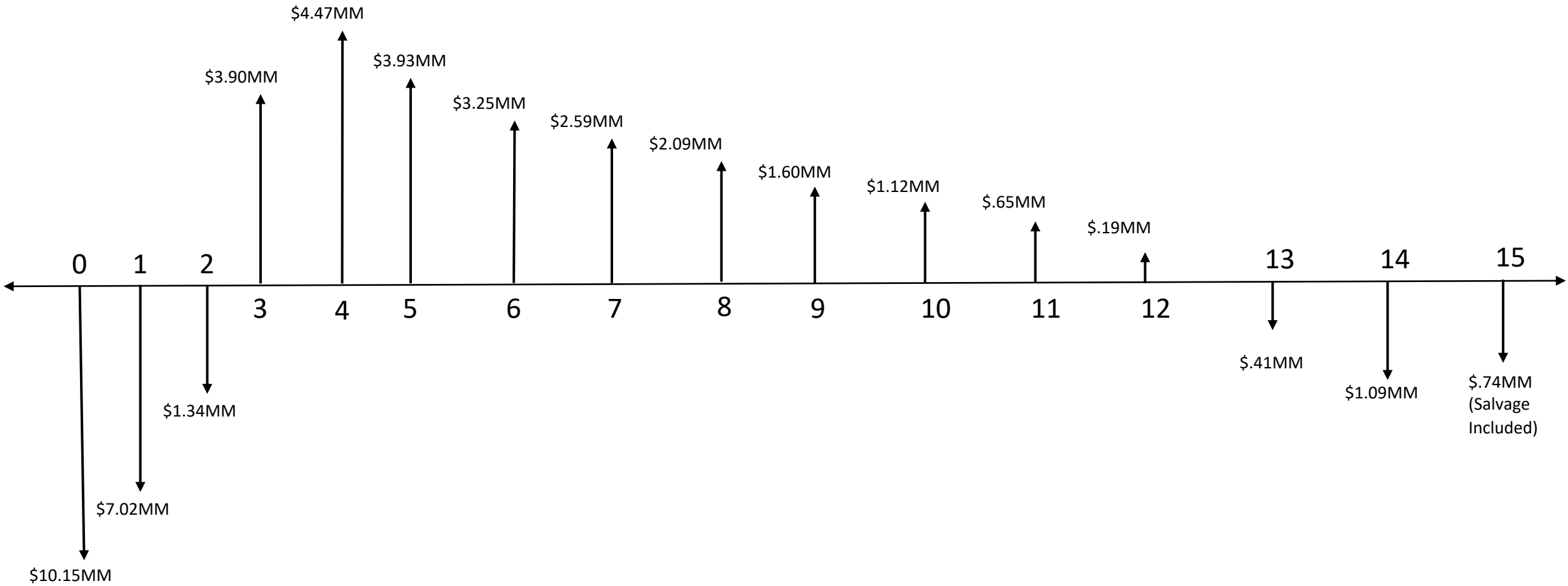


ECONOMICS

Economic Analysis

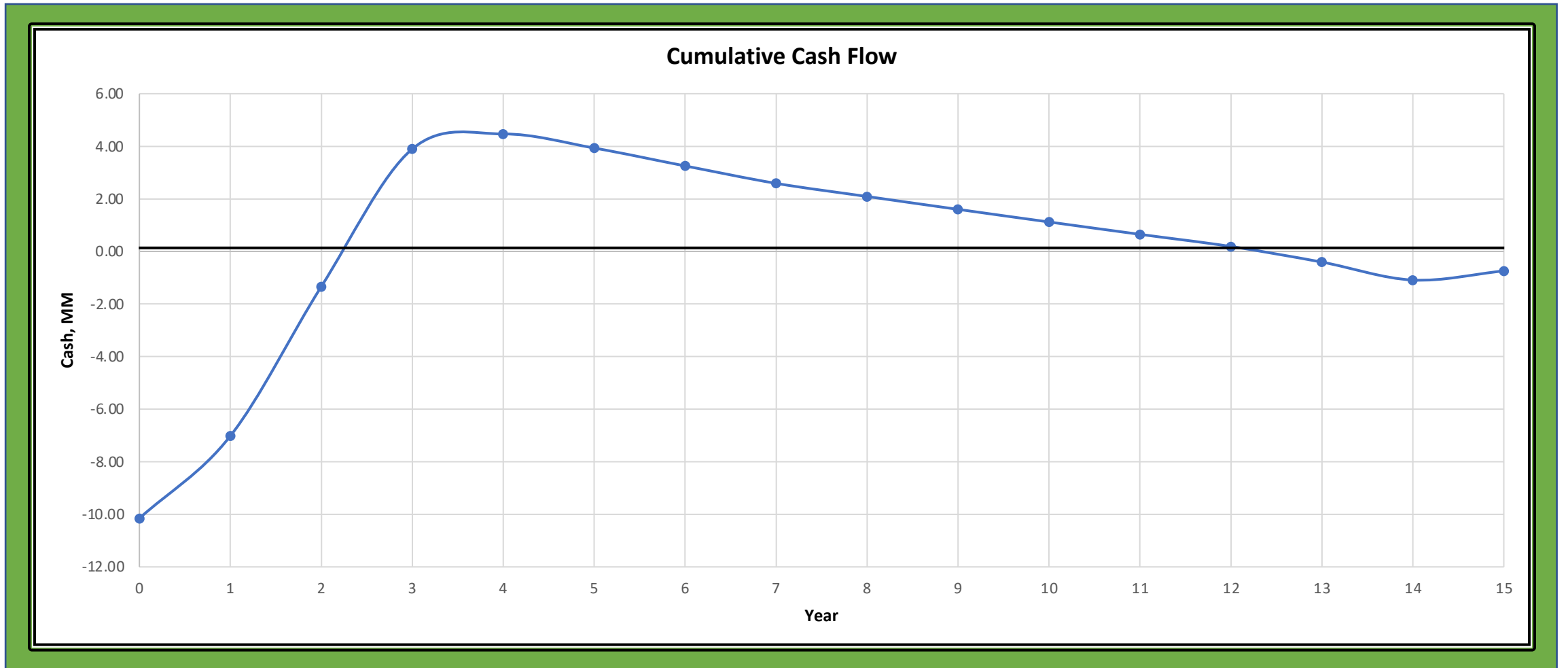
Economic Evaluation	
Total Capital Investment, 10^6	\$10.2
Annual Total Production Costs, 10^6	\$34
Annual Sales, 10^6	\$37
Payback Period, yrs	4.2
Return on Investment, %/year	22
Discounted Cash Flow Rate of Return, %/yr	13
Net Present Value, 10^6	\$8
Salvage Value, 10^6	\$1
Cumulative profit, 10^6	\$23

TCI Cash Flow Diagram



*Assume 2% TPC Inflation Rate + Depreciation

Cash Flow



SAFETY

PROCESS SAFETY HOLDING & HANDLING

HOLDING

Dimethyl Ether

- Keep away from heat
- Equipment must be grounded
- Store in a cool, well-ventilated area
- Keep away compressed oxygen or strong oxidizers
- Stored between 7-14 bar & up to 52°C

Methanol

- Methanol maximum exposure of 200 ppm (OSHA & EPA)
- Tightly closed container
- Well –ventilated area.
- Equipment must be grounded and bonded.

HANDLING

- Use of ventilators and breathing protection or local exhaust.
- The use of cold-insulating gloves.
- Oversee the use of Personal Protective Equipment (PPE).



SAFETY CONSIDERATIONS

Factor	Consideration
Markings and Labelling	Clear indications of toxicity and flammability reports on equipment at the plant. Toxicity (Exposure limits) - 1900 mg/m ³ , 1000 ppm. ("Dimethyl ether", 2021) NFPA Flammability no. - 4
Waste disposal	Determination of toxicity and physical properties to determine the proper waste classification and disposal methods.
Container disposal	Draining the containers thoroughly and venting in a safe place away from fire and sparks. Critical temperature – 126.9°C ("Dimethyl ether", 2021) Auto-ignition temperature - 350°C
Local Legislation	Waste disposal in accordance with local, regional and national laws and regulations

Safety Guidelines in Accordance with Rules and Regulations of Plaquemine, Louisiana

Pre-Line Opening Job Preparations

- The shutting down and energy isolation of all process systems prior to any line opening involving process piping, equipment or vessels (4.1.1).
- The draining and/or depressurization of all process piping, equipment or vessels to ensure clearance of hazardous materials (4.1.2).
- Ensuring temperatures for the process piping, equipment or vessels have sufficiently cooled to allow for safe work (4.1.3).

Line Opening Job Planning

- The barricading of affected areas with a minimum of 10 ft radius as a precautionary area (4.2.1.1)
- The issuance of permits strictly by authorized personnel (4.2.2.1)



HAZARD ANALYSIS T-102 FEED LINE

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the feed line	There is pressure build up in the feed line leading into the tower	-Blockage in the system	- Failure of feed line tube - Risk of expansion of column and bursting	Installation of quick-pressure relief valves at strategic locations before and after the column.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in feed line	There are sudden pressure losses in the streams leading to the column	- Leakages in the system	- Insufficient reactant material entering the column	Pressure alarms at the feed, distillate and bottom streams	- Installation of pressure gauge - Checking maintenance schedule and procedures
2	Flow	Reverse	Backflow from T-102	The contents of the tower flow back to the feed line	- Clogging and blockages within the tower	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow - Following the stipulated maintenance schedule and procedures
3	Temperature	More	Increase in feed temperature	There is sudden increase in temperature at the feed of T-102	- Clogging of inlet into tower	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at feed entry point. - Panel alarms to warn of high pressure or temperature	-Installation of a temp gauge - Checking maintenance schedule and procedures

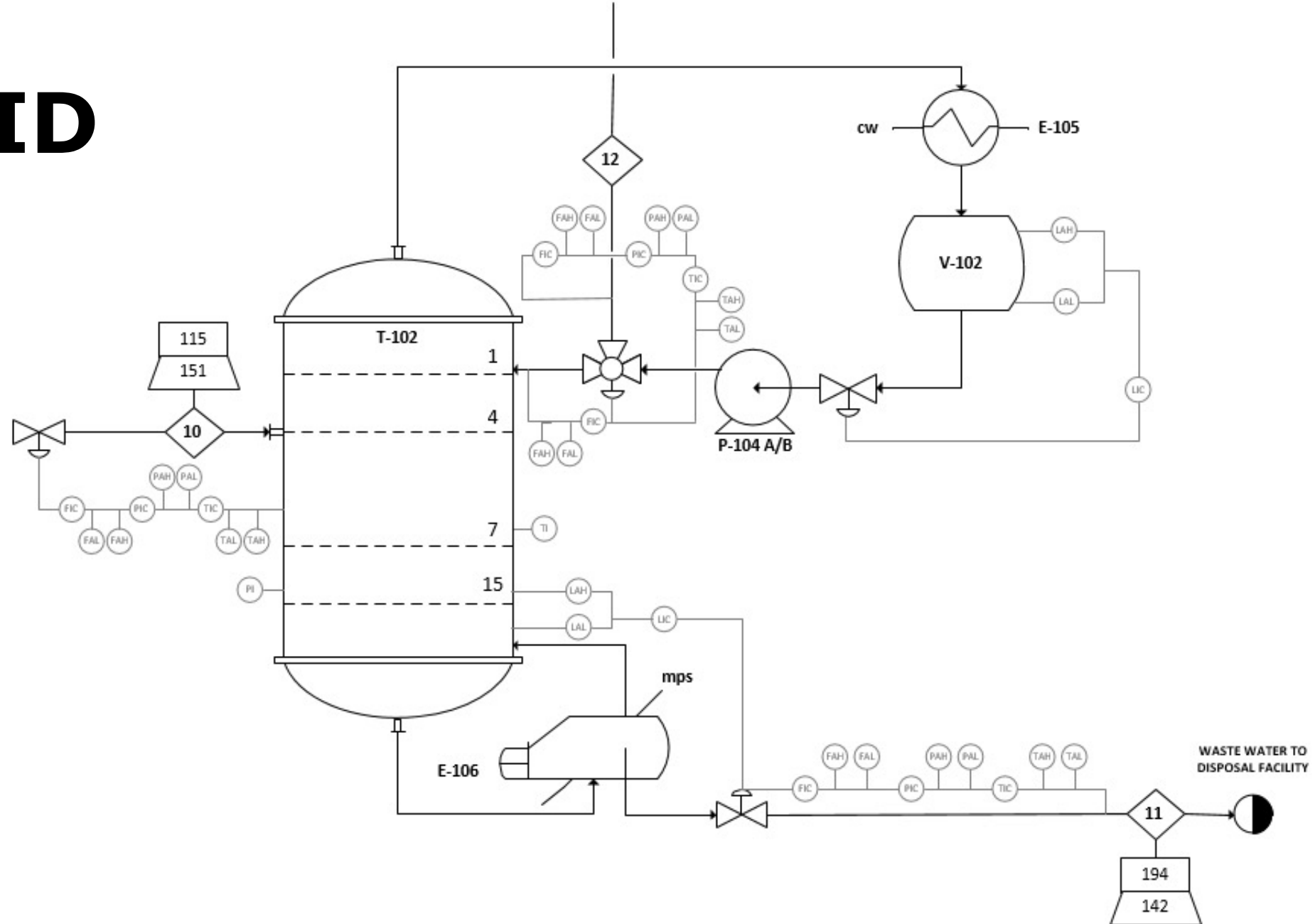
HAZARD ANALYSIS T-102 DISTILLATE LINE

No.	Parameter	Guideword	Deviation	What if ?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the distillate line	There is pressure build up in the distillate line transporting recycled methanol to the mixer	-Blockage in the mixer or further up the distillation line	- Failure of distillate line tube - Risk of expansion of mixer and bursting. - Failure of mixer	Installation of quick-pressure relief valves at strategic locations before the mixer.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in feed line	There are sudden pressure losses in the stream leading to the mixer	- Leakages in the distillate line	- Inefficiencies within the tower leading to less methanol distillate	Pressure alarms at the exit of the column where the distillate line begins.	- Installation of pressure gauge - Checking maintenance schedule and procedures
2	Flow	Reverse	Backflow to T-102	The contents of the distillate line flow back to the tower	- Clogging and blockages within the line	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow- Following the stipulated maintenance schedule and procedures
3	Temperature	More	Increase in distillate line temperature	There is sudden increase in temperature at distillate line transporting recycled methanol	- Clogging of inlet into the mixer	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at mixer entry point. - Panel alarms to warn of high pressure or temperature	-Installation of a temp gauge - Checking maintenance schedule and procedures

HAZARD ANALYSIS T-102 BOTTOM LINE

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the bottom line	There is pressure build up in the bottom-line transporting wastewater to treatment plant	-Blockages within bottom line	- Failure of bottom-line tube - Risk of expansion and bursting of the line.	Installation of quick-pressure relief valves at strategic locations within the line.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in bottom line	There are sudden pressure losses in the stream within the bottom line leading away from the tower	- Leakages in the bottom line	- Inefficiencies within the tower causing decreased flow of wastewater from the tower	Pressure alarms at the exit point from the tower joining the bottom line	- Installation of pressure gauge - Checking maintenance schedule and procedures
2	Flow	Reverse	Backflow to T-102	The contents of the bottom-line flow back to the tower	- Clogging and blockages within the line	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow - Following the stipulated maintenance schedule and procedures
3	Temperature	More	Increase in bottom line temperature	There is sudden increase in temperature at bottom line transporting wastewater to the treatment plant	- Clogging of the line at various points	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at exit point of the tower to the bottom line. - Panel alarms to warn of high pressure or temperature	-Installation of a temp gauge - Checking maintenance schedule and procedures

P&ID



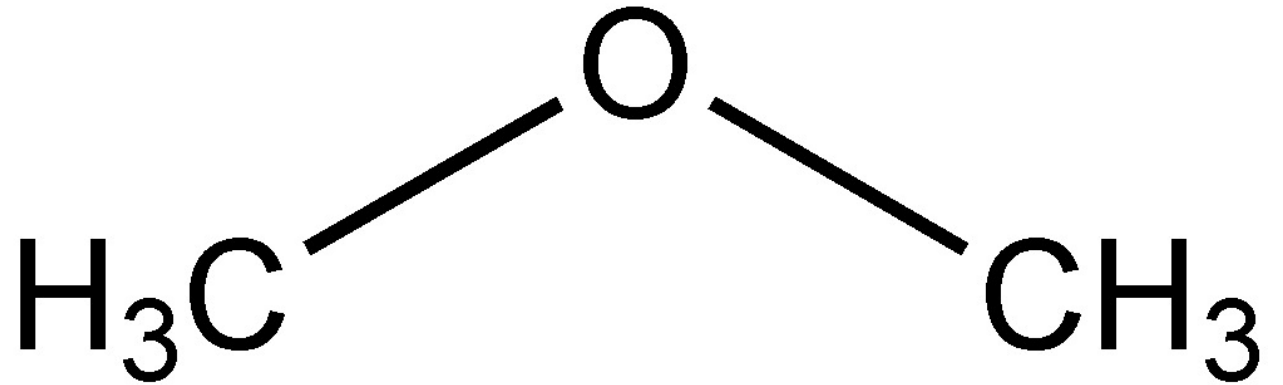


WASTEWATER TREATMENT

- Reduce Pollutants in Water
 - Negative health effects on life species
- Useful for all aspects of life
 - Irrigation or Recreational Use
- Send Wastewater to SNF Holding Company
 - Plaquemine Facility

CONCLUSION

- Methanol Dehydration To Form DME
- 99.9% Purity DME
- 90% Plant Utilization (329 Days)
- Collect Salvage After Year 12
- \$23MM Profit, 22% ROI
- Recommend Pursuing Design



ACKNOWLEDGEMENTS

Dr. Emmanuel Dada

Dr. Lealon Martin

Industrial Advisory Counsel

Roy G. Perry College of Engineering Faculty & Staff

Thank you!

QUESTIONS?

APPENDIX

REFERENCES

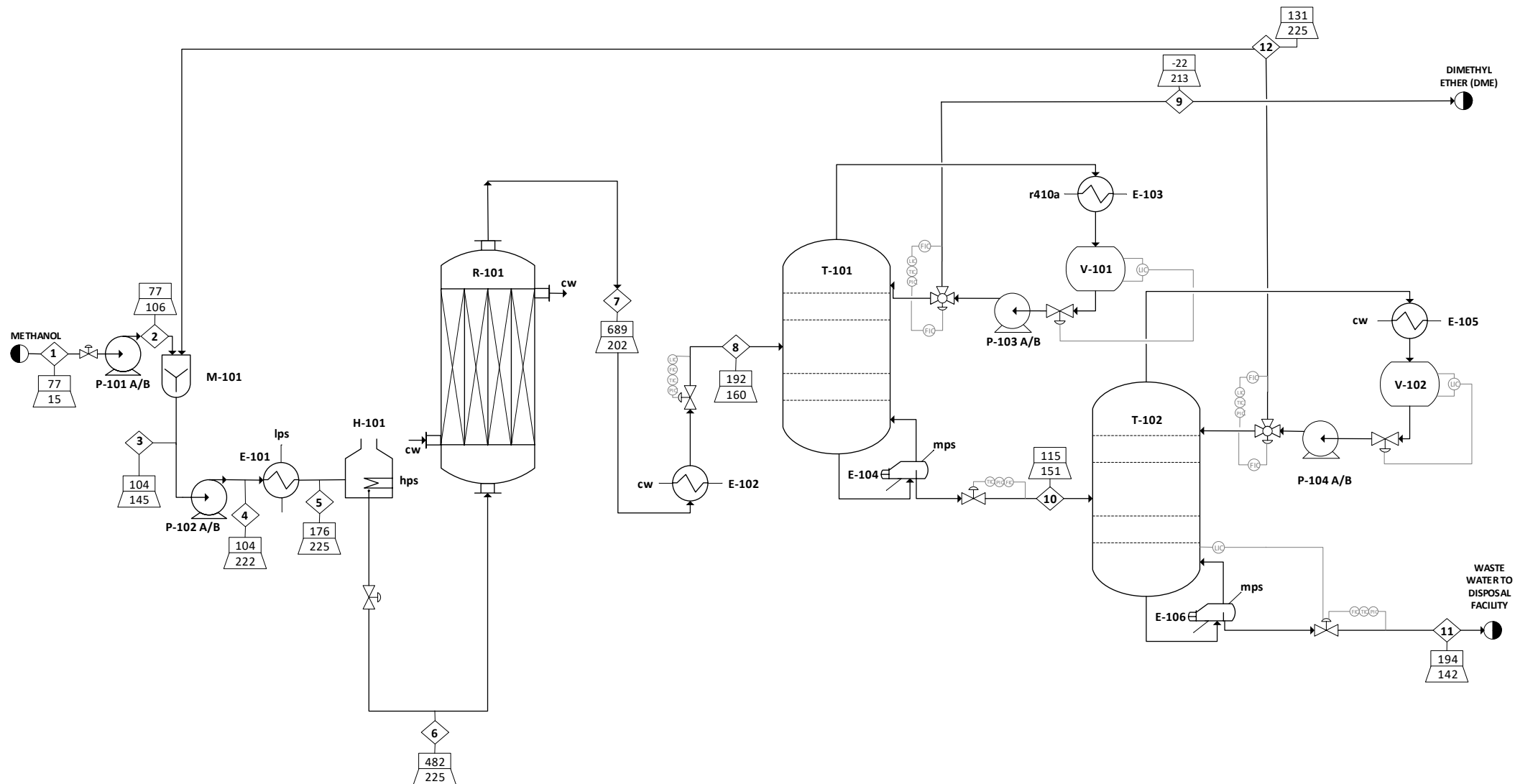
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STOICHIOMETRY



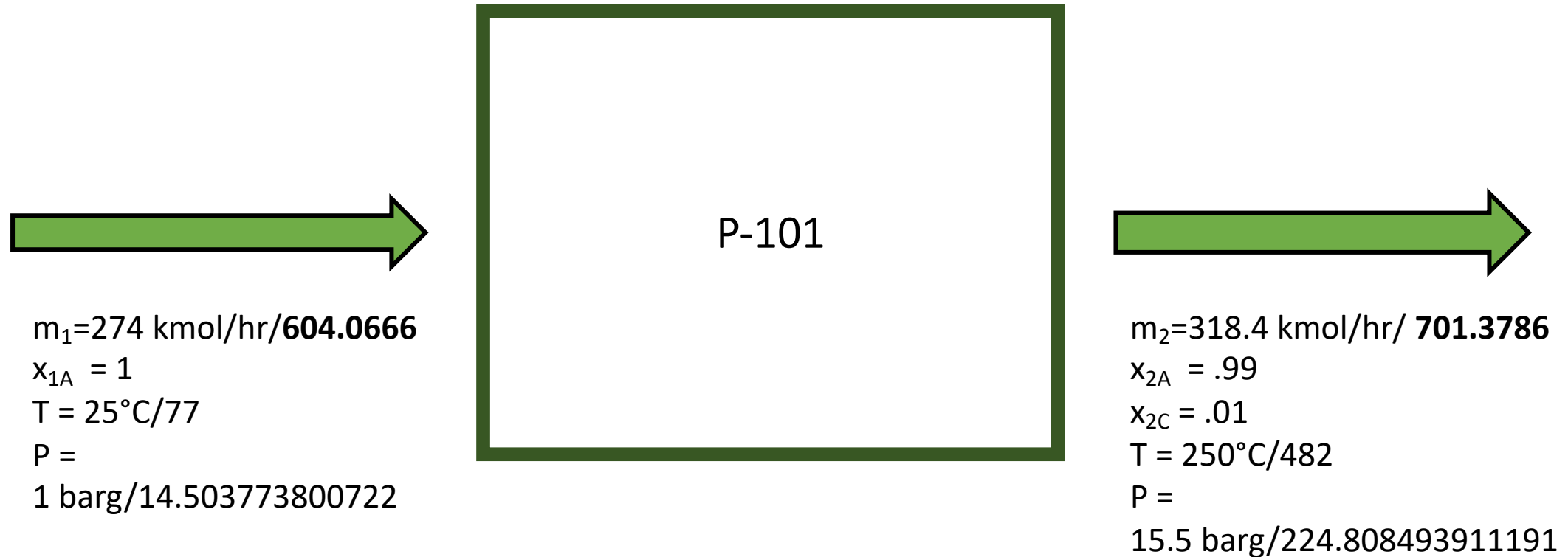
	A (Methanol)	B (Dimethyl Ether)	C (Water)
lb-mol	2	1	1
Molecular Weight lb/lbmol	32.04	46.07	18

P-101 A/B Feed Pump	M-101 Fresh & Recycled Methanol Mixer	P-102 A/B Combined Feed Pump	E-101 Methanol Vaporizer	H-101 Fired Heater	R-101 Methanol Catalytic Packed Bed Reactor	E-102 DME Cooler	T-101 DME Distillation Tower	E-103 T-101 Condenser	E-104 T-101 Reboiler	V-101 T-101 Reflux Drum	P-103 A/B T-101 Reflux Pump	T-102 Methanol Distillation Tower	E-105 T-102 Condenser	E-106 T- 102 Reboiler	V-102 Methanol Reflux Drum	P-104 A/B T-102 Reflux Pump
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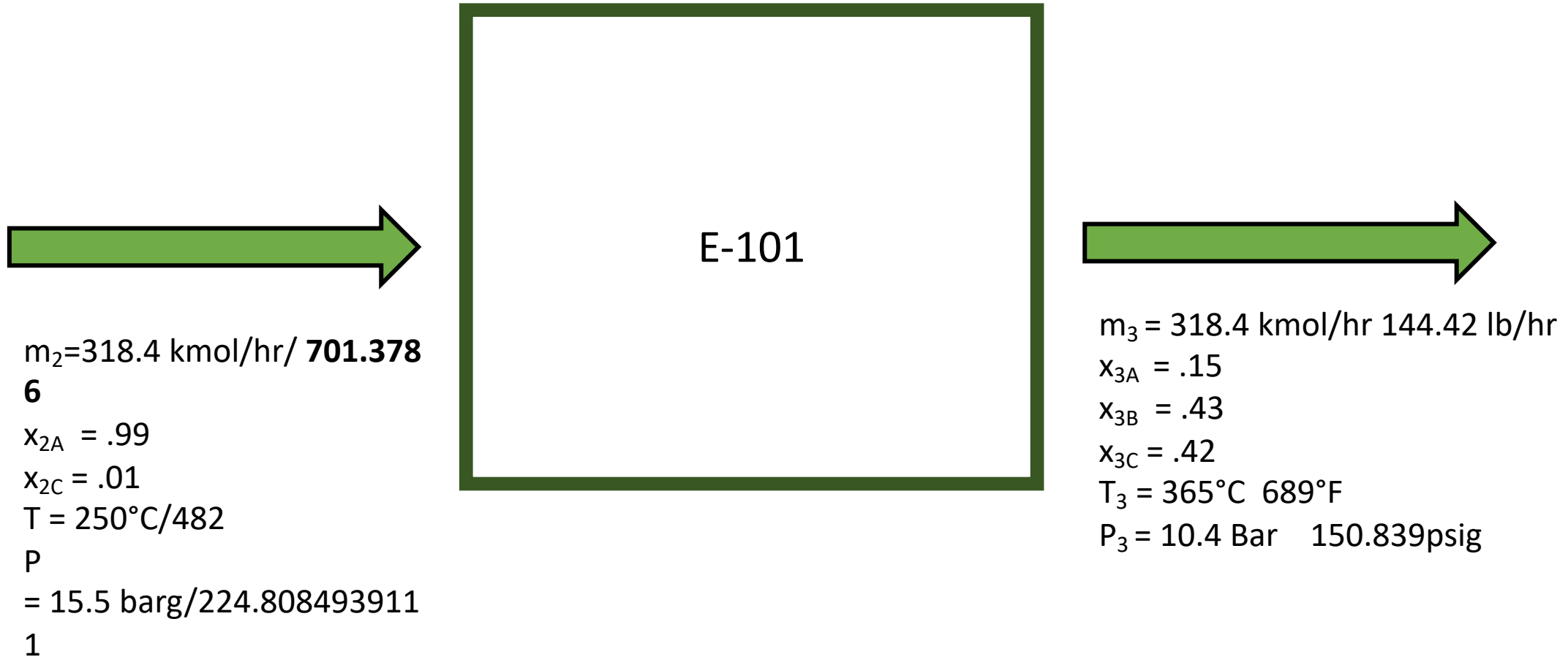


 Temperature, °F
 Pressure, psig

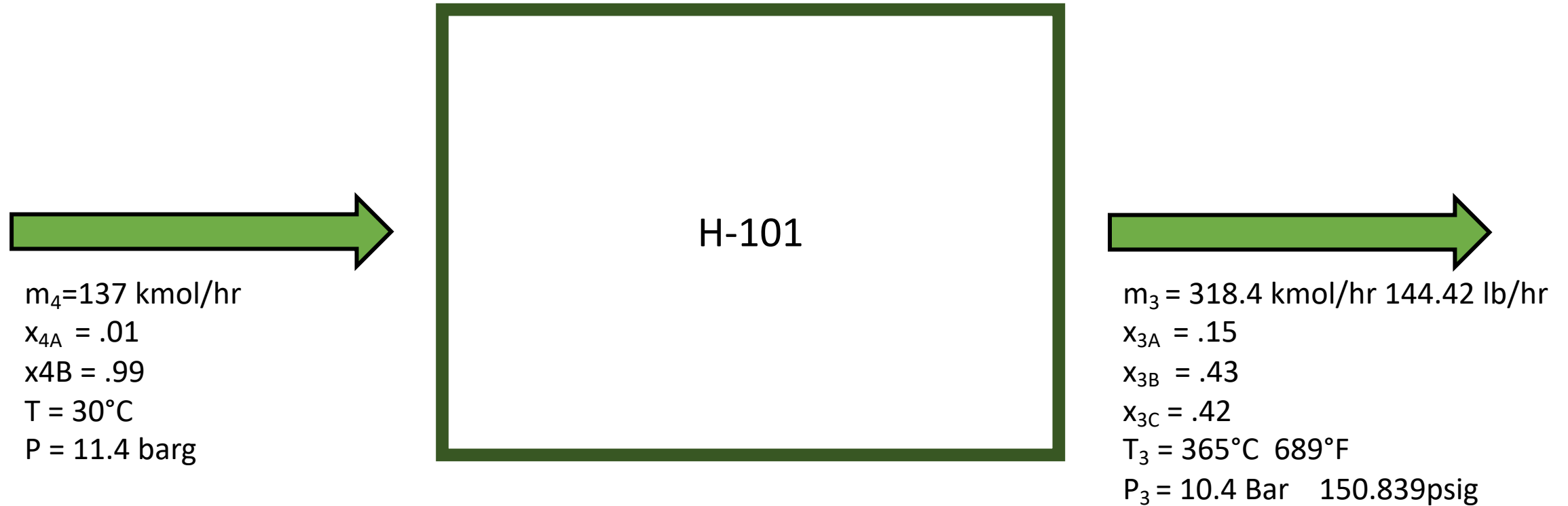
Pump Material Balance



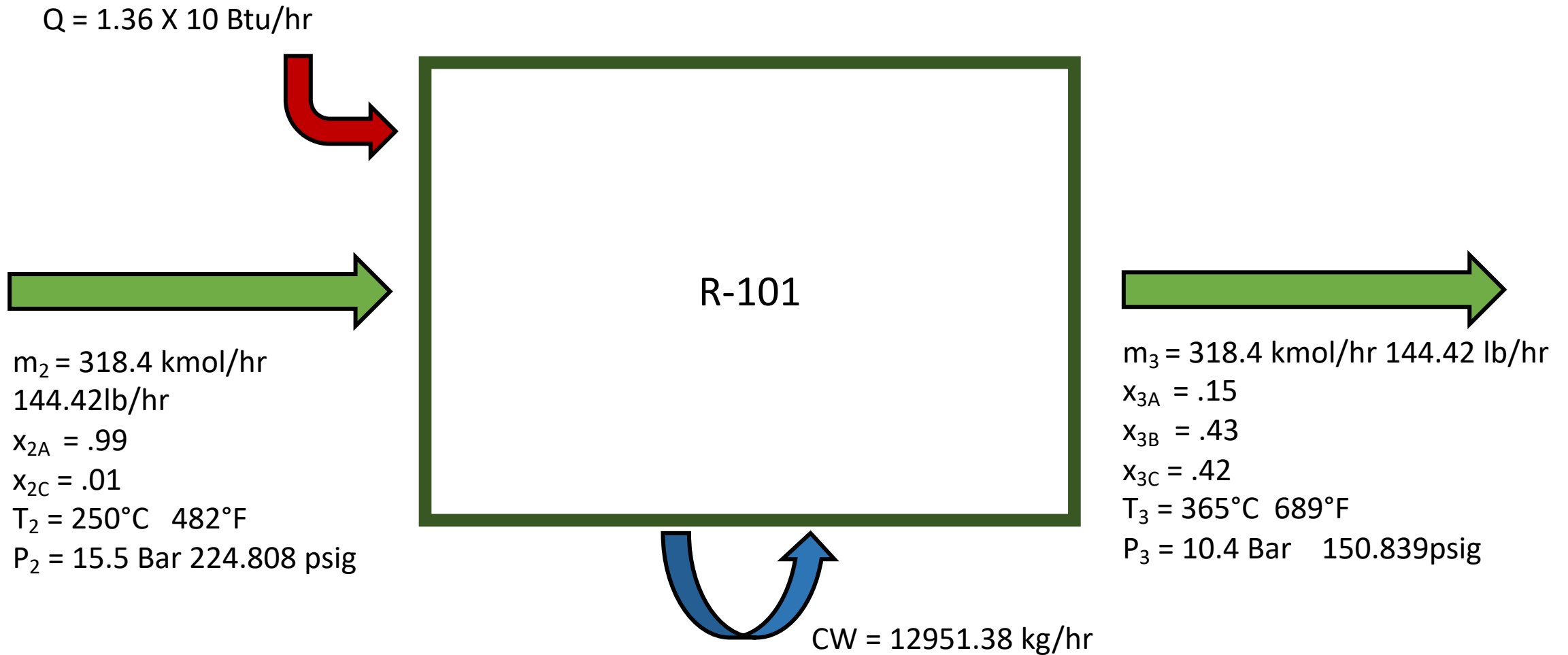
Vaporizer Material Balance



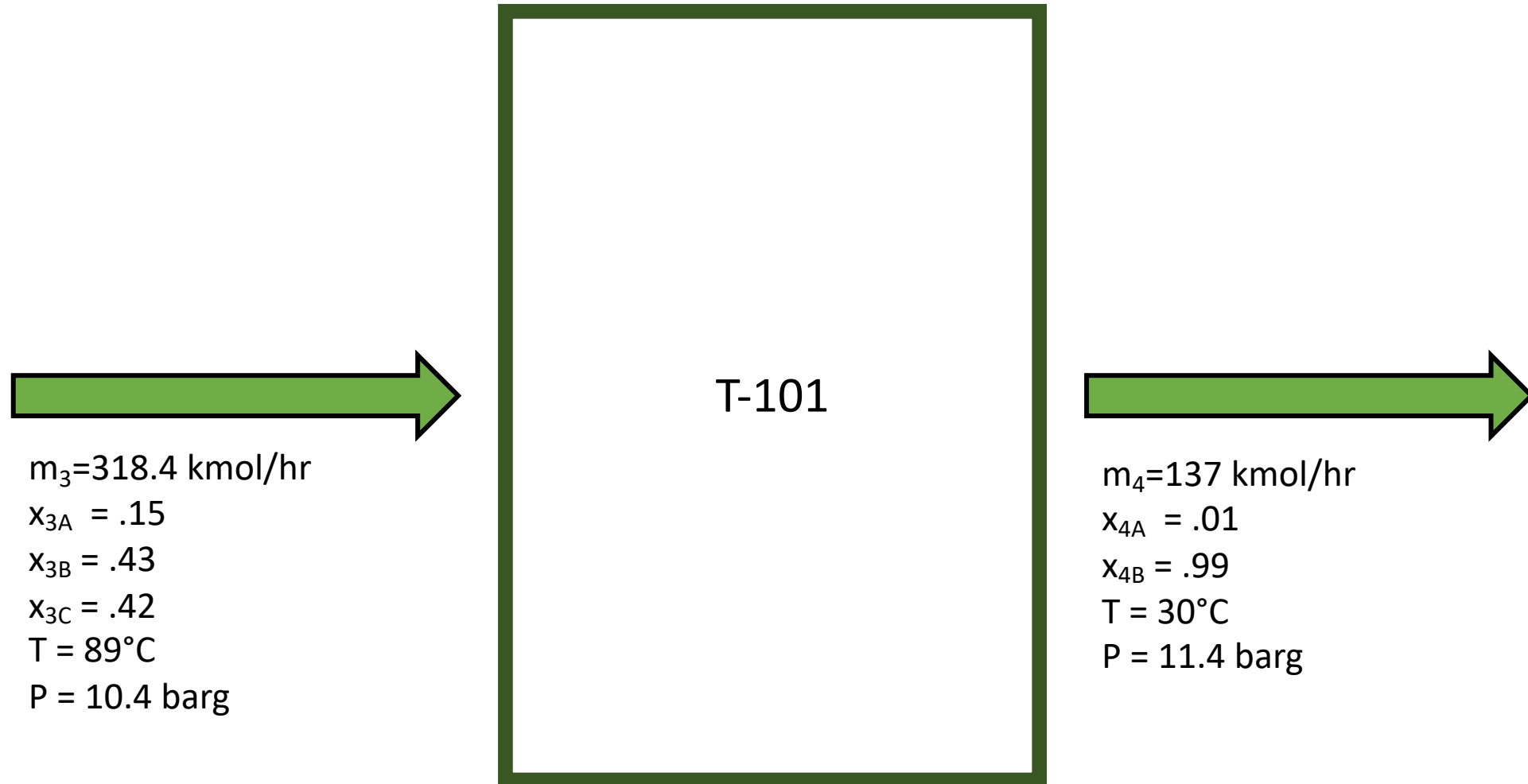
Furnance Material Balance



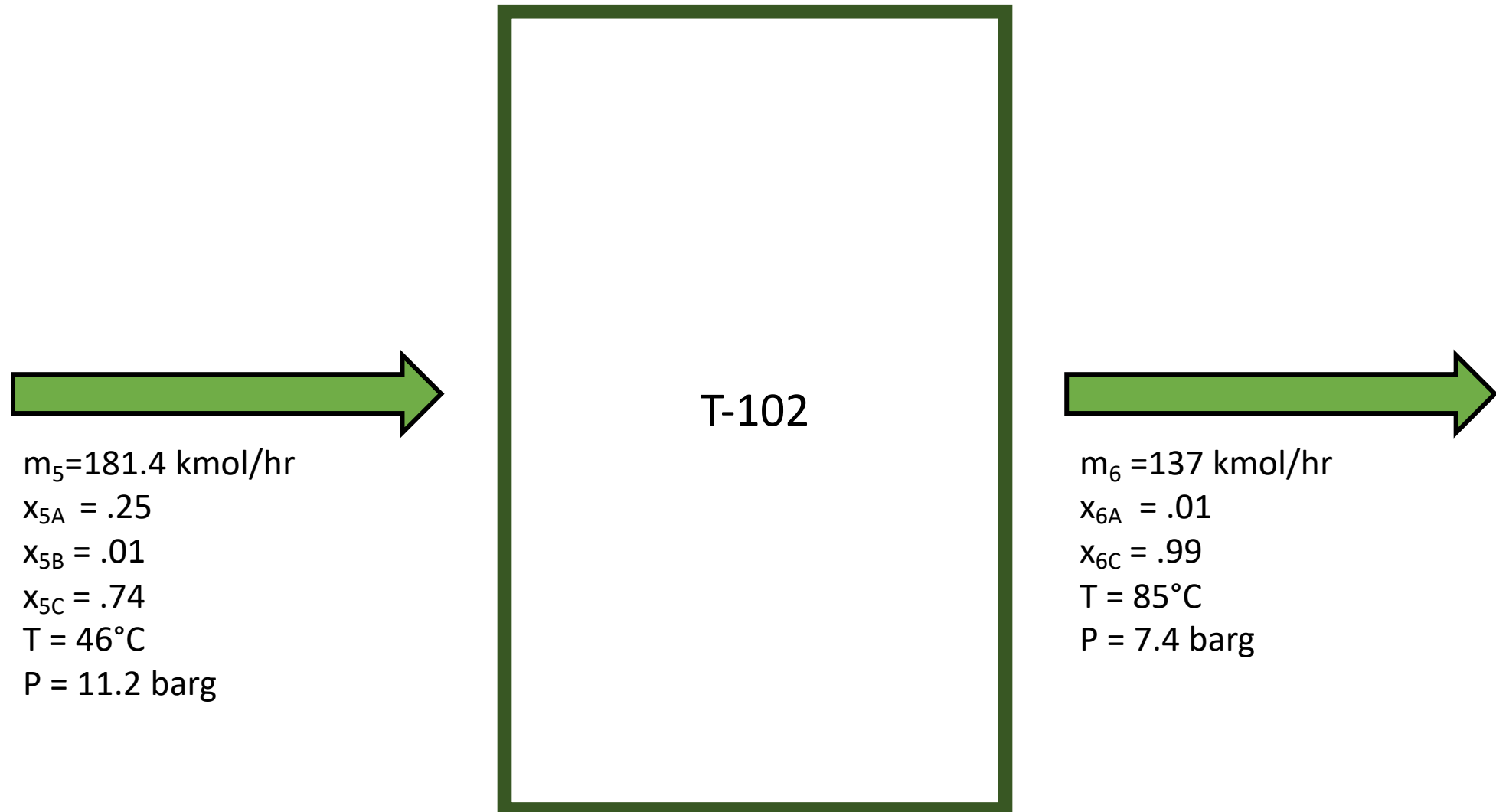
Dehydration Reactor Material Balance



1st Distillation Column Material Balance

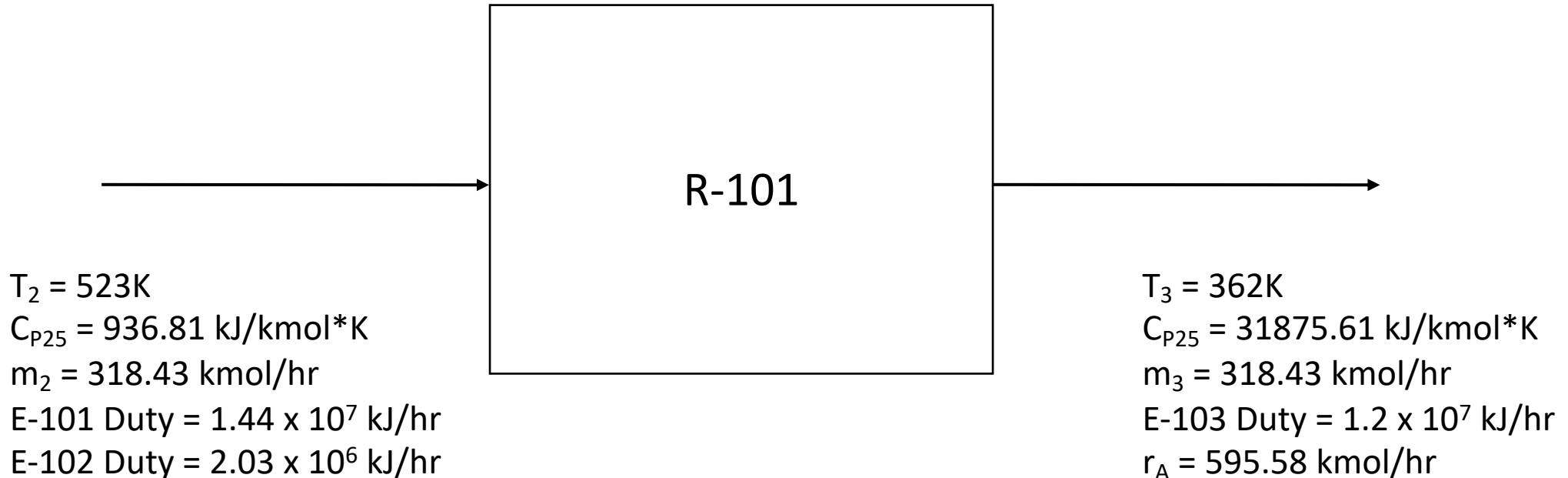


2nd Distillation Column Material Balance



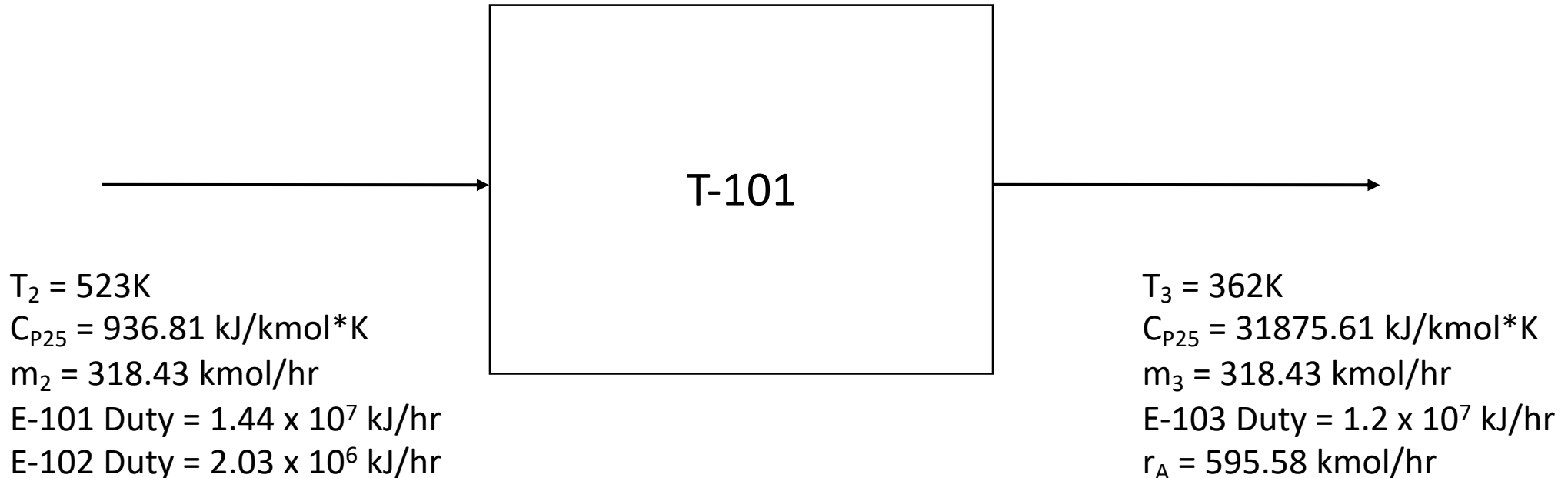
ENERGY BALANCE

$$\Delta H_{\text{RXN } 280} = -5.9 \times 10^6 \text{ kJ/kmol}$$



ENERGY BALANCE

$$\Delta H_{\text{RXN } 138} = -5.9 \times 10^6 \text{ kJ/kmol}$$



ENERGY BALANCE

Stream	1	2	3	4	5	6	7	8	9	10	11
Molar Enthalpy (kJ/kmol)	-238400	-238305	-201079	-200560	-164896	-198934	-234554	-179812	-239321	-280413	-233583
Mass Enthalpy (kJ/kg)	-7440.2	-7437.2	-6275.5	-6263.1	-3579.3	-6212.3	-7324.6	-3915.0	-12513.8	-15445	-7321.9
Molar Entropy (kJ/kmol*K)	-240.2	-239.9	-150.1	-148.6	-211.9	-120.2	-206.5	-244.2	-162.9	-148.7	-213.1
Mass Entropy (kJ/kg*K)	-7.5	-7.5	-4.7	-4.6	-4.6	-3.8	-6.4	-5.3	-7.6	-8.2	-6.7

R-101 Design Equations

$$\textcircled{1} \text{ Mole Balance: } F_{A0} \frac{dx}{dw} = -r'_A = \frac{\text{kg mol}}{\text{kg cat} \cdot \text{hr}}$$

$$\textcircled{2} \text{ Rate Law: } -r'_A = k C_A^2 = \frac{\text{kg mol}}{\text{kg cat} \cdot \text{hr}}$$

$$\textcircled{3} \text{ Stoichiometry: } C_A = \frac{C_{A0}(1-x)}{1+\epsilon x} \frac{P}{P_0} \frac{T_0}{T}, \quad \frac{P}{P_0} = p \quad (\text{pg. 169})$$

$$\begin{aligned} \frac{dp}{dw} &= -\frac{\alpha}{2p} (1+\epsilon x) \frac{T_0}{T} \\ \frac{T_0^2 p}{T} \frac{dp}{dw} &= -\alpha \\ \frac{T_0^2 p^2}{T} \frac{dp}{dw} &= -\alpha \quad (\text{pg. 174}) \end{aligned}$$

$$\textcircled{4} \text{ Combine: } \frac{dx}{dw} = \frac{k C_{A0}^2 (1-x)^2}{F_{A0} (1+\epsilon x)^2} \left(\frac{P}{P_0} \right)^2 \left(\frac{T_0}{T} \right)^2 = \text{kg cat}^{-1}$$

R-101 Design Equations

$$Q = UA\Delta T_{lm} f_r$$

$$Q = \dot{m} C_p \Delta T$$

$$T_{HIN} = 250^\circ\text{C}$$

$$T_{HOUT} = 305^\circ\text{C}$$

$$T_{CIN} = 30^\circ\text{C}$$

$$T_{COUT} = 45^\circ\text{C}$$

$$\dot{m} = 318.43 \text{ kmol/hr}$$

$$\dot{m} = 318430 \text{ mol/hr}$$

$$C_p = 110 \text{ J/mol K}$$

$$\Delta T = 305 - 250 = 115 + 273$$

$$= 388 \text{ K}$$

$$Q = \dot{m} C_p \Delta T$$

$$= 318430 \frac{\text{mol}}{\text{hr}} (110 \frac{\text{J}}{\text{mol K}}) (388 \text{ K})$$

$$Q = 1.433 \times 10^{10} \text{ J/hr}$$

$$U = 500 \text{ BTU/hr-ft}^2\text{ }^\circ\text{F}$$

$$\Delta T_{lm} = 204.7^\circ\text{C} \rightarrow 508.46^\circ\text{F}$$

$$f_r = 1.0$$

$$Q = 1.433 \times 10^{10} \text{ J/hr}$$

$$Q = 13582219.3 \text{ BTU/hr}$$

$$Q = UA\Delta T_{lm} f_r$$

$$A = \frac{Q}{U\Delta T_{lm} f_r}$$

$$= \frac{13582219.3 \text{ BTU/hr}}{(500 \frac{\text{BTU}}{\text{hr-ft}^2\text{ }^\circ\text{F}}) (508.46^\circ\text{F}) (1.0)}$$

$$A = 53.425 \text{ ft}^2$$

$$A = 4.963 \text{ m}^2$$

Tubes: $A_T = \pi D L$, $n = A/A_T$

$$D = 1.060 \text{ in} = 0.02667 \text{ m}$$

$$L = 14.477 \text{ ft} = 4.479 \text{ m}$$

$$A_T = (3.14) (0.02667 \text{ m}) (4.479 \text{ m})$$

$$A_T = 0.375 \text{ m}^2$$

$$n = \frac{A}{A_T} = \frac{4.963 \text{ m}^2}{0.375 \text{ m}^2}$$

$$n = 13.2 \approx 14 \text{ Tubes}$$

$$W = 24923 \text{ Kg cat}$$

$$1790.214 \text{ Kg cat per Tube}$$

$$\frac{Q}{A\Delta T_{lm} f_r} = U$$

$$\frac{13582219.3 \text{ BTU/hr}}{(107.039 \text{ ft})(508.46^\circ\text{F})(1)}$$

$$U = 248.167 \frac{\text{BTU}}{\text{hr-ft}^2\text{ }^\circ\text{F}}$$

$$U = 200 \frac{\text{BTU}}{\text{hr-ft}^2\text{ }^\circ\text{F}} \left(\begin{array}{l} \text{within} \\ \text{range} \end{array} \right)$$

$$A = \frac{13582219.3 \text{ BTU/hr}}{(200 \frac{\text{BTU}}{\text{hr-ft}^2\text{ }^\circ\text{F}}) (508.46^\circ\text{F}) (1.0)}$$

$$A = 133.56 \text{ ft}^2$$

$$A = 12.408 \text{ m}^2$$

T-101 Design Equations

Water: 100°C

$$N_{min} = \frac{\ln \left[\left(\frac{x_{1k}}{x_{2k}} \right)_D \left(\frac{x_{1k}}{x_{2k}} \right)_B \right]}{\ln \alpha_{1k}}; \alpha_{1k} \approx 9 \text{ (Research)}$$

$$= \frac{\ln \left[\left(\frac{.99}{.01} \right) \left(\frac{.25}{.01} \right) \right]}{\ln(9)} = 3.5 \approx 4$$

R_{min} : $q = 0.0$ for saturated vapor (Perry's 13-36)

$$1 - q = \sum_j \frac{\alpha_{jk} x_{jk,F}}{\alpha_{jk} - \phi} \quad \leftarrow \text{Underwood equation}$$

$$\alpha_{1k} - \phi = \alpha_{1k} x_{1k,F}$$

$$\phi = \alpha_{1k} - \alpha_{1k} x_{1k,F} = \alpha_{1k} (1 - x_{1k,F}) = 5.13 \quad \checkmark$$

Underwood constant
 $1 < \phi < \alpha_{1k}$

$$R_{min} = \sum_j \frac{\alpha_{jk} x_{jk,D}}{\alpha_{jk} - \phi} - 1$$

$$= \frac{9 \cdot .99}{9 - 5.13} - 1 = 1.3$$

$$R/R_{min} = 1.2 - 1.3 \text{ (pg 235 in short cut design book)}$$

$$\therefore R = (R_{min})(1.3) = 1.7$$

$\leftarrow$ Gilliland correlation

Number of theoretical trays (pg 236 short cut book)

$$\frac{R - R_{min}}{R + 1} = \frac{1.7 - 1.3}{1.7 + 1} = .15 \quad \therefore \text{use chart on left}$$

$$@ .15, \quad \frac{N - N_{min}}{N + 1} = .45$$

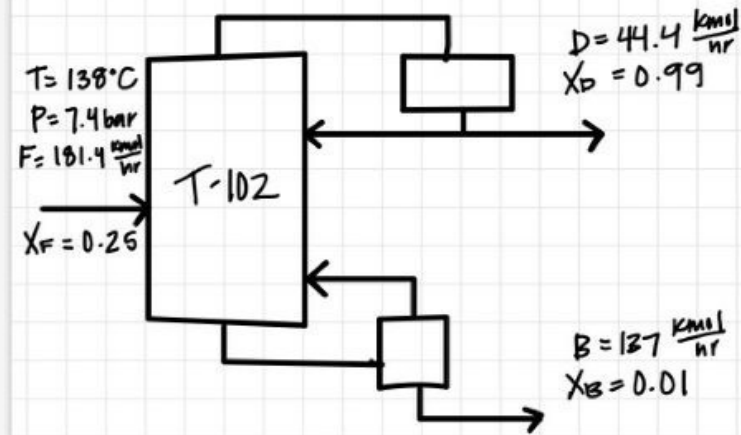
$$.45N + .45 = N - N_{min}$$

$$N_{min} + .45 = .55N$$

$$N = \frac{N_{min} + .45}{.55} = \frac{4.45}{.55} = 8.09 \approx 9$$

$$N/N_{min} = 1.8 - 2.5 = 8/4 = 2.25 \quad \checkmark$$

T-102 Design Equations



Rectifying

$$y_{N+1} = \frac{R}{R+1} X_N + \frac{X_D}{R+1}$$

$$y_{N+1} = \frac{4.472}{4.472+1} X_N + \frac{0.99}{4.472+1}$$

$$y_{N+1} = 0.817 X_N + 0.181$$

↳ rectifying operating line

Stripping

Feed: $X_F = 0.25$

$T = 411 \text{ K}$

$P = 7.4 \text{ bar}$

$$y = \frac{q}{q-1} X - \frac{X_F}{q-1} ; q = \frac{H_V - H_F}{H_V - H_L}$$

$$u = \frac{0.05}{0.05-1} X - \frac{0.25}{0.05-1} \rightarrow y = -0.05 X + 0.24$$

↳ stripping operating line

q-line

$$q = \frac{H_V - H_F}{H_V - H_L} = \frac{2704.24 - 2053.42}{2704.24 - 700.885}$$

$q = 0.05$

Interpolate

$$\begin{aligned} H_L &= 703.241 & y_1 &= 703.241 & y_2 &= 709.301 \\ X_1 &= 725 \text{ KPa} & X_2 &= 750 \text{ KPa} \end{aligned}$$

$$y = 703.241 + (740 - 725) \left(\frac{709.301 - 703.241}{750 - 725} \right)$$

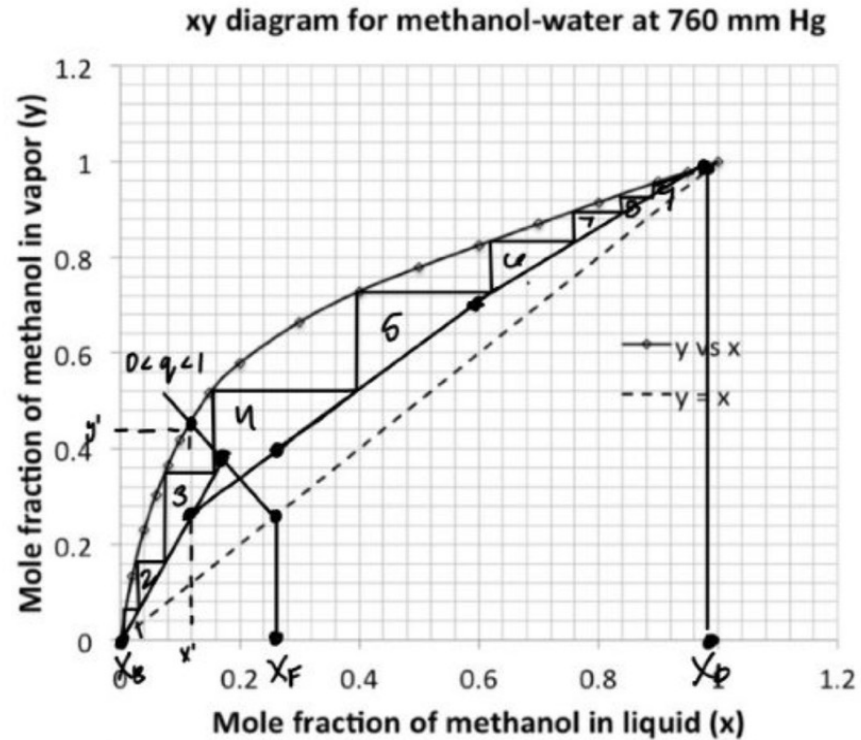
$$H_L = 700.885 \text{ kJ/kg}$$

$$\begin{aligned} H_V &= 2703.4 & y_1 &= 2703.4 & y_2 &= 2704.8 \\ X_1 &= 725 \text{ KPa} & X_2 &= 750 \text{ KPa} \end{aligned}$$

$$H_V = 2704.24 \text{ kJ/kg}$$

$$H_F = 2053.42 \text{ kJ/kg}$$

T-102 Design Equations



$$x' = 0.1$$

$$y' = 0.3$$

$$\text{SDL: } y = -0.05x + 0.26$$

$$\text{ROL: } y_{n+1} = 0.917x_n + 0.191$$

$$9 + 1 = \underline{10 \text{ stages}}$$

Minimum Reflux Ratio

$$\frac{R_m}{R_m + 1} = \frac{x_D - y'}{x_D - x'} \xrightarrow{\text{pinch point}} \frac{0.99 - 0.3}{0.99 - 0.1} = 0.775$$

$$\frac{R_m}{R_m + 1} = 0.775 \rightarrow R_m = 0.775R_m + 0.776 \rightarrow 0.225R_m = 0.775 \rightarrow \underline{R_m = 3.44}$$

Reflux Ratio

$$1.3 = \frac{R}{R_{\min}}$$

$$\underline{R = 4.472}$$

EPA & OSHA Regulations

OSHA (Methanol)

- The sampling group
- The sampling time at 60 min.
- The sampling volume at 3 L or 5L when humidity is greater than 50%

EPA (Methanol)

- Occupational exposure through inhalation.
- Exposure through the ambient air from its evaporation during solvent uses.
- Acute effects by inhalation and/or ingestion resulting in blurry vision and disorientation.
- Chronic effects including insomnia, elevated levels of liver enzymes and decreased brain weight.

EPA (DME)

- Tolerance exemptions that are associated with Dimethyl Ether (DME)
- Regulations of the emission standards associated with DME



Total Capital Investment

Direct Costs	
Purchased equipment, E'	1.496
Delivery, fraction of E'	0.150
Subtotal: delivered equipment	1.646
Purchased equipment installation	0.773
Instrumentation&Controls(installed)	0.592
Piping (installed)	1.119
Electrical systems (installed)	0.181
Buildings (including services)	0.296
Yard improvements	0.165
Service facilities (installed)	1.152
Total direct costs	5.924
Indirect Costs	
Engineering and supervision	0.543
Construction expenses	0.675
Legal expenses	0.066
Contractor's fee	0.362
Contingency	0.724
Total indirect costs	2.370
Fixed capital investment (FCI)	8.294
Working capital (WC)	1.465
Total capital investment (TCI)	9.758

Utilities

Steam		
LPS	MPS	HPS
\$1.16MM	\$.355MM	\$.392MM
TOTAL		\$1.91MM/yr

Cooling Water	
Amount Required, ft ³ /yr	9.92 x 10 ⁶
TOTAL	\$14,000/yr

Electricity	
Amount Required, kWh/yr	1.06 x 10 ⁵
TOTAL	\$5,000/yr

Wastewater Disposal	
Amount Required, ft ³ /yr	7.03 x 10 ⁵
TOTAL	\$11,000/yr

Refrigerant, r140a	
Amount Required, BTU/yr	4.10 x 10 ⁸
TOTAL	\$5,000/yr

Materials & Labor

Raw Materials		
Name of Material	Price, \$/lb	Annual Amount MM kg/year
Methanol	.16	~71
TOTAL		\$25.28MM/yr

Labor		
Number of Operators per Shift	Shifts Per Day	Operator Rate, \$/hr
3	3	34
TOTAL		~\$1MM/yr

Product		
Name of Material	Price, \$/lb	Annual Amount MM kg/year
DME	.41	50
TOTAL		\$45MM/yr

EMISSIONS

- The use of DME reduces carbon emissions by an average of 25%.
- DME synthesis from methanol is a low carbon footprint process.
- The total final emissions are negative at an estimate of **-39 ktCO₂eq per year**

Process stream	Units	Value
Methanol	KgCO _{2eq} /t	-1643
Wastewater	KgCO _{2eq} /t	500

ASPEN STREAM TABLES

Stream	Methanol	Recycle*	DME + Methanol + Water	Methanol + Water	DME	Recycle	Water
Mole Flows kmol/hr	274	44.4	318.4	177.13	141.27	34.72	142.01
Mass Flows kg/hr	8779.55	1416.44	10196	3687.81	6508.18	1117.85	2569.96

AVERAGE

**Average Student Original Graded Assignment on Final Project
Powerpoint Presentation**

Production of 1,3 Butadiene From Ethanol



JAM CHEMICAL
• CHEMICAL PLANT •

Instructor: Dr. Dada

Senior Design I

84%

83%

83%

85%

85%

Group 1: Mohamed Akinotcho, Duaa Al Badri, Cayla Alexander, Jevaun Christie, Au'Myia Collins



PROBLEM STATEMENT

- Design a 1,3 Butadiene production plant utilizing the Ostromislensky reaction that is capable of producing and purifying 200,000 tons of butadiene annually from local ethanol feedstock.
- Develop a profitable production process to convert ethanol to 1,3-Butadiene with 98% purity.

PROJECT GOALS

DESIGN A PLANT FOR THE PRODUCTION OF 1,3-BUTADIENE (BD)

Objective	Criteria	Units of Measurement
Determine Plant Capacity	Demand Gap	Production/ Year
Produce Monomer Grade BD (98%)	Purity	Mass Composition
Produce BD within Environmental and Safety Constraints	EPA & OSHA Regulations	Parts Per Million
Maximize positive margin between Feedstock and Products	Product Sold - Feedstock Cost	Dollars/Year

WHO ARE WE?

VISION- To deliver effective and efficient products to our stakeholders and consumers.

MISSION- Committed to providing the highest quality precision products and service to the plant industry.

LOCATION- Corpus Christi, Texas

GANTT CHART

1,3 Butadiene to Ethanol Plant Design

smartsheet

	Tasks	Assigned To	Duration	Start Date	End Date
1	Literature Search		10 days	09/21/21	10/01/21
2	Project Selection		2 days	09/21/21	09/22/21
3	Initial Research		8 days	09/23/21	10/04/21
4	Process Selection		9 days	10/05/21	10/15/21
5	Process & Reaction		8 days	10/05/21	10/14/21
6	Flowsheet Development		33 days	10/15/21	11/30/21
7	Basic Information		7 days	10/15/21	10/23/21
8	Process Flow Diagram Draft		21 days	10/25/21	11/22/21
9	Material Energy and Balances		110 days	11/22/21	03/12/22
10	ASPEN HYSYS		21 days	02/13/22	03/06/22
11	Identify Process		2 days	02/14/22	02/15/22
12	Converge Process		8 days	02/16/22	02/24/22
13	Results of Stimulation		9 days	02/25/22	03/06/22
14	Major Equipment Specifications		28 days	02/02/22	03/02/22
15	Design of each Major Equipment		21 days	02/03/22	02/23/22
16	Detailed Information		7 days	02/24/22	03/02/22
17	Economic Analysis		22 days	03/09/22	03/31/22
18	Capcost		7 days	03/09/22	03/16/22
19	Cost Evaluation		7 days	03/17/22	03/24/22
20	Develop Cash Flow		7 days	03/25/22	03/31/22
21	Reporting		207 days	09/21/21	04/16/22
22	Selecting Process		2 days	09/21/21	09/22/21
23	Homework Assignments		198 days	09/21/21	04/09/22
24	Midterm Progress Report		TBD	TBD	03/07/22
25	End of the semester Report		86 days	01/20/22	04/16/22
26	End of semester Presentation		86 days	01/20/22	04/16/22

OUTLINE

- BACKGROUND
- PLANT METRIC
- MARKET ANALYSIS
- PLANT CASH FLOW DIAGRAM
- SUMMARY OF ECONOMICS
- PROCESS SELECTION
- PROCESS CHEMISTRY
- PROCESS FLOW DIAGRAM
- MATERIAL BALANCE
- ENERGY BALANCE
- ASPEN SIMULATION
- SPECIFICATION SHEET
- SAFETY & HANDLING

BACKGROUND

HOW IT USED?

ETHANOL:

- Gas
- Corn
- Plastics
- Topical Medicine
- Cosmetics



1,3 BUTADIENE:

- Plastics
- Resin
- Rubber
 - Latex
 - Nitrile
 - Styrene Butadiene



PROPERTIES OF 1,3 BUTADIENE

Molecular Formula	C_4H_6
Molecular Weight	0.12lb/mole
Normal Boiling Point	24 °F
Melting Point	-162°F
Critical Temperature	306°F
Critical Pressure	627 Psi
Liquid Pressure	41 lb/ft ³
Appearance	Colorless non-corrosive gas or refrigerated liquid
Odor	Gasoline-like odor

PLANT METRIC

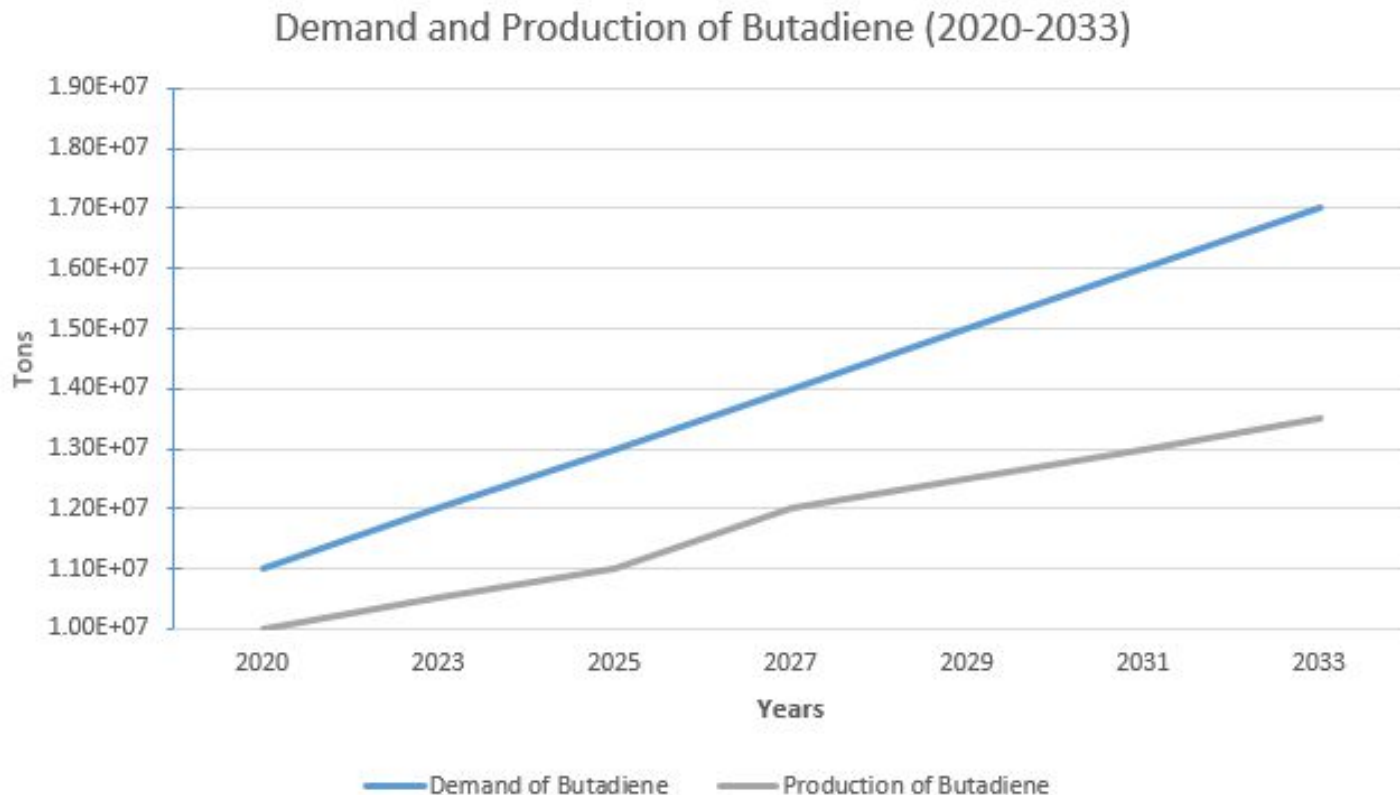
(Capacity & Location)

KEY METRICS

- Raw material used to produce 1,3 Butadiene is ethanol.
- Capacity 200,000 tonnes of butadiene per year from ethanol.
- Location decided to produce product in Texas.



GLOBAL BUTADIENE PRODUCTION AND DEMAND



PLANT CAPACITY COMPARISON

COMPANY	LOCATION	CAPACITY (tons)
ExxonMobil Chemical Company	Baton Rouge, Louisiana	162,600
Shell Chemical LP	Deer Park, Texas	180,000
Equistar Chemicals, LP	Channelview, Texas	432,657
INEOS	Germany	350,000
JAM CHEMICAL	CORPUS CHRISTI, TEXAS	200,000

PLANT LOCATION

LOCATION- Corpus Christi, Texas

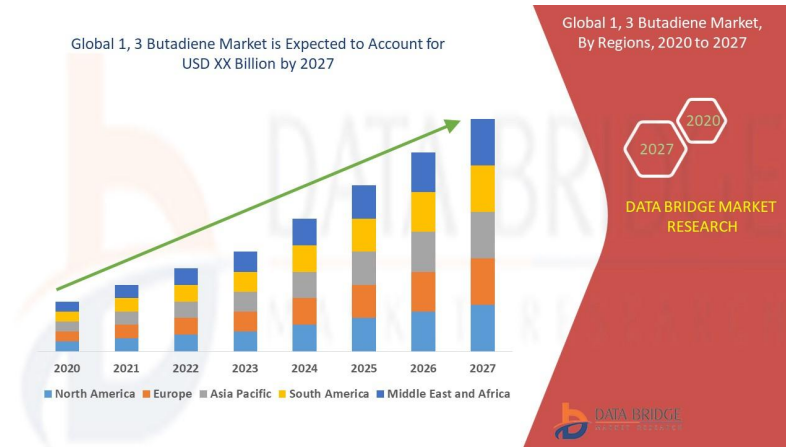
- Close to large body of water
- Nearby Interstate Grain Corporation deep water export facility and ADM deep water export facility
- Transportation of Raw Materials:
 - Railroad
 - Ocean Vessels
 - Tanker Trucks



MARKET ANALYSIS

MARKET ANALYSIS

- Global 1,3 butadiene market by type (extractive distillation , Oxidative dehydration)
- Will reach an estimated valuation of 19.6 million tons by 2027 while registering this growth at a rate of 4.50% for the forecast period of 2020-2027 as data bridge market research

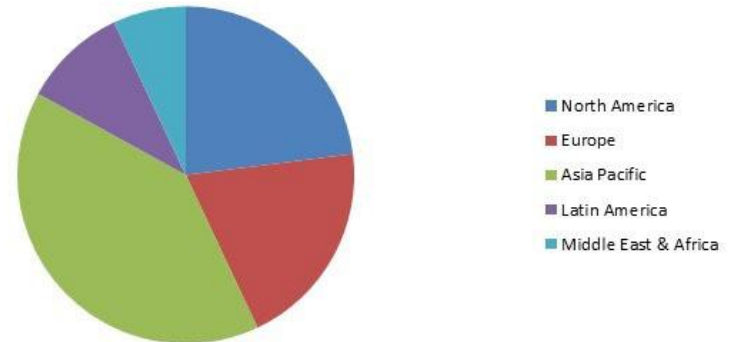


MARKET ANALYSIS

The major players covered in 1,3 butadiene market report are :

- BASF SE
- Exxon Mobil
- Lyondellbasell industries
- China cooperation
- Royal Dutch shell
- Sabic
- LG chem
- Bangkok synthetic
- Chevron phillips chemical company
- Formosa plastic corporation
- Reliance industries limited
- INEOS
- Dow
- Braskem
- Air liquide

Global 1,3 Butadiene Market Share (%)- By Region-2016



Source: Research Nester

CONSUMER OF 1,3 BUTADIENE

CLIENT SELECTION:

- Goodyear Tire & Rubber
- Dow Chemical
- Firestone Synthetic Rubber & Latex
- Lanxess
- Ameripol Synpol
- Michelin
- Perelli
- Bridgestone

BRIDGESTONE



GOODYEAR



LANXESS
Energizing Chemistry

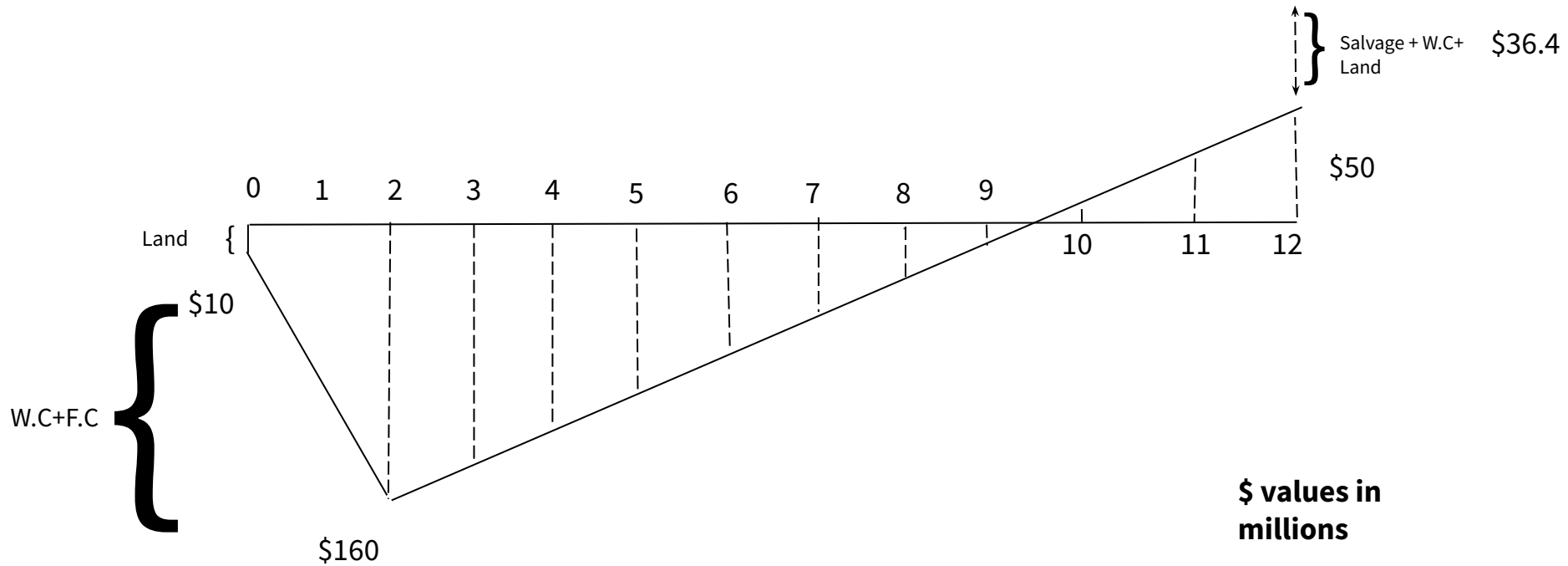


Firestone



PLANT CASH FLOW DIAGRAM

Cash Flow



SUMMARY OF ECONOMICS

Cash Flow Analysis

Net Present Value (NPV)	(\$30,964,090.78)
Investor's Rate of return	3%
Payback Period (yrs)	7.619
Fixed Capital Investment (FC)	\$136,000,000
Working Capital (WC)	\$24,000,000
Land	\$10,000,000

PROCESS SELECTION

PROCESS SELECTION

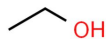
PRODUCTION ROUTES	PROS	CONS
Extraction from C4 hydrocarbons	Cheap raw material	High operating cost Low selectivity Non sustainable Toxic
Dehydrogenation of n-butane	Cheap raw material	Low selectivity Less sustainable
Ethanol ✓	Cheap raw material Non toxic Biorenewable Environmental Friendly	Endothermic reaction requires high heating utilities
n-Butanol	Biorenewable	Endothermic reactions requires high heating utilities & Low selectivity

ONE STEP PROCESS VS TWO STEP PROCESS

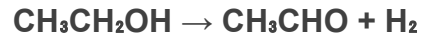
PROCESSES	PROS	CONS
ONE STEP (IPATIEV Process)	Low complexity reactions	Higher capital costs due to multiple reactors
TWO STEP (OSTROMYSLENSKY) Process ✓	Higher % Yield (18%) 98% Purity Less energy consumed due to lower reaction temperature	Limited process optimization High Energy consumption

PROCESS CHEMISTRY

Chemical structures/ information about each compound

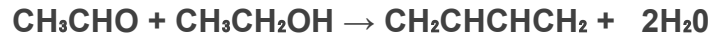
	Ethanol	Acetaldehyde	Hydrogen Gas	1,3 Butadiene	Water
Molecular Weight	0.1016lbs/mol	0.097 lbs/mol	2.016 lb/lbmol	54.09 lb/lbmol	0.040 lbs/mol
Chemical Formula	C ₂ H ₆ O	C ₂ H ₄ O	H ₂	CH ₂ CHCHCH ₂	H ₂ O
Chemical Structure					
Boiling Point	78.39°C (173.1°F)	20.2°C (68.36°F)	-252.89°C (-423.2°F)	-4.4°C (24.08°F)	37.78°C (100°F)
Freezing Point	-173.5 F -114.1 C	-190.3 F -123.3 C	-434.5 F -259.2 C	-164 F -108.9 C	32 F 0 C
Flash Point	12.0 °C c.c	-38°C c.c.	Flammable gas	-76°C c.c	N/A
Critical Temperature	513.9 C	183 C	33.2C	161.8 C	374 C
Auto- Ignition Temperature	400°C	185°C	560°C	414°C	N/A

PROCESS CHEMISTRY



- ❑ In the first step of the process, ethanol reacts over a heterogeneous catalyst, copper-chromite, to form acetaldehyde and hydrogen with 92% selectivity on a shell-and-tube, packed bed reactor.
- ❑ The chosen catalyst in the first reaction, copper-chromite, has detailed kinetic parameters for dehydrogenation, allowing operating conditions to be optimized by simulation. Optimization for the first reactor was focused on obtaining an ethanol conversion of 50%. 50% was chosen because it minimized the amount of ethanol required for the entire process, without unnecessary waste.
- ❑ A significant amount of hydrogen is produced through the first reaction, and thus a process of separating and purifying the hydrogen is also required.
- ❑ The separated hydrogen is used as fuel for utility heat.

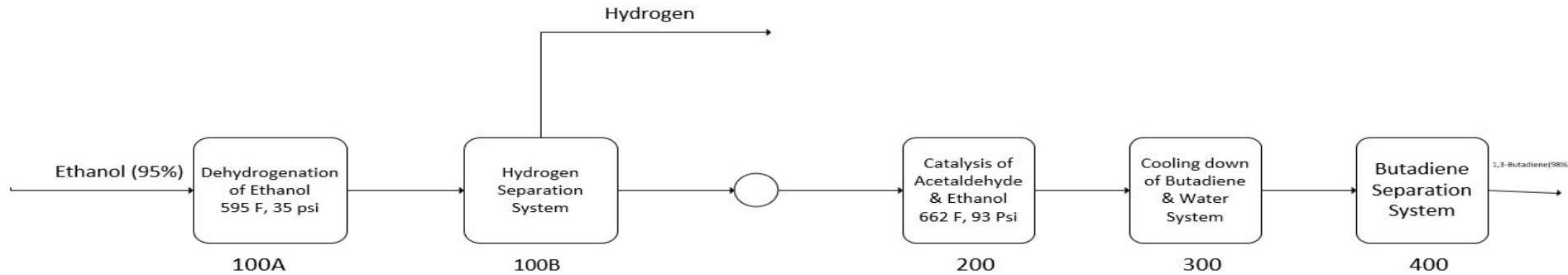
PROCESS CHEMISTRY



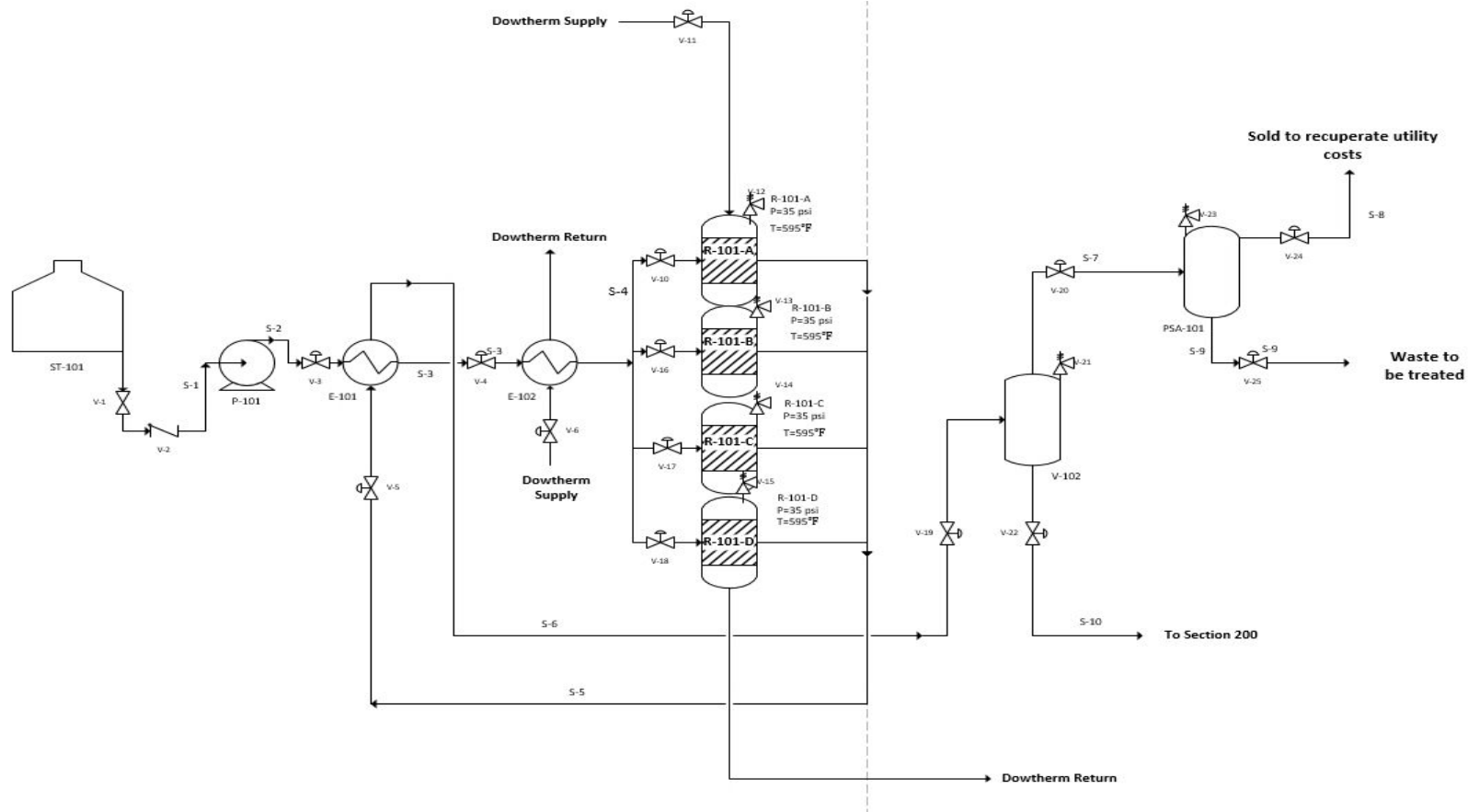
- ❑ In the second step of the Process Acetaldehyde is mixed with ethanol to form butadiene and water in a heterogeneous tantalum-silica catalyst with 55% selectivity on same type of reactor as the first reaction.
- ❑ Finally, this last product goes through a distillation train to separate our final product 1,3 Butadiene from the byproduct and recycle feeds, ethanol and acetaldehyde.

PROCESS FLOW DIAGRAM

BLOCK FLOW DIAGRAM



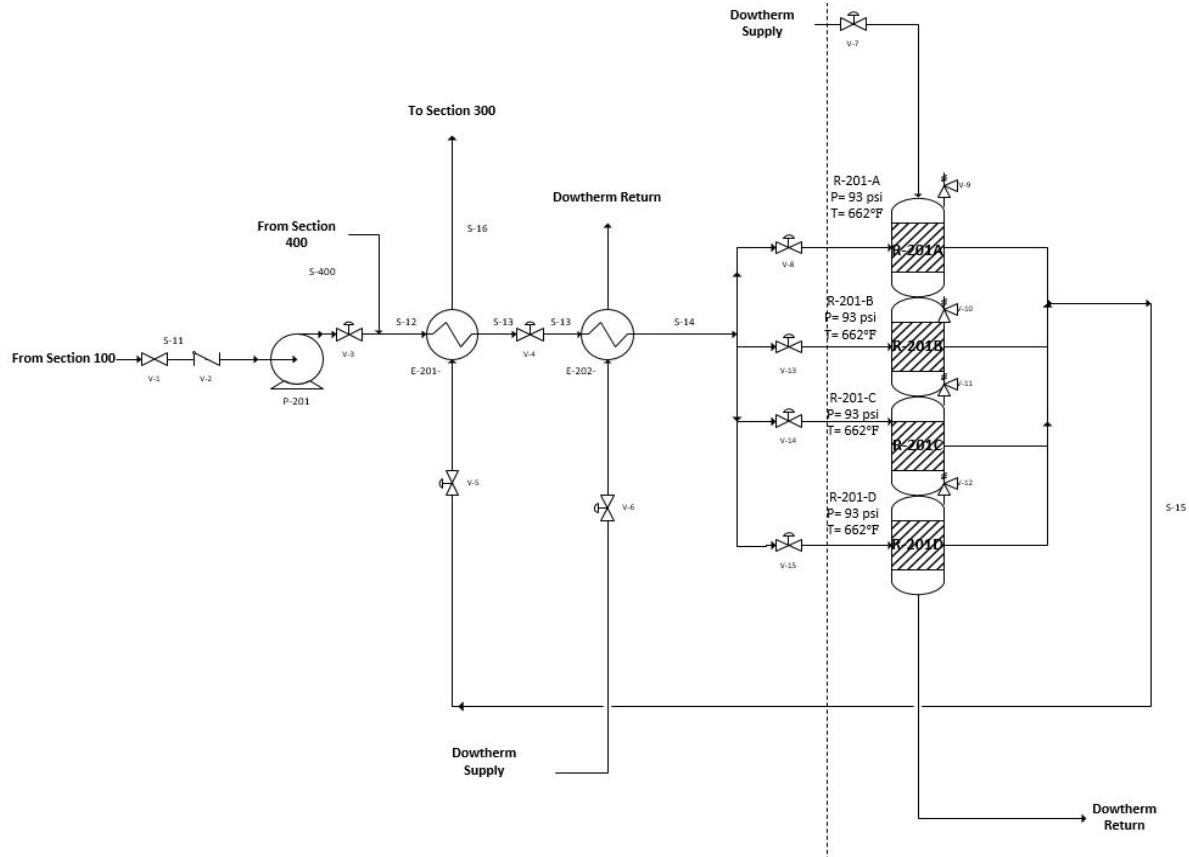
SECTION 100



SECTIONS 100 STREAMS

Stream	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
Phase	Liquid	Liquid	Mixed	Vapor	Vapor	Mixed	Vapor	Vapor	Mixed	Mixed
Temp.(°F)	80	80	226	595	595	152	121	121	121	121
Pressure (psi)	15	50	42	35	30	22	155	155	155	155

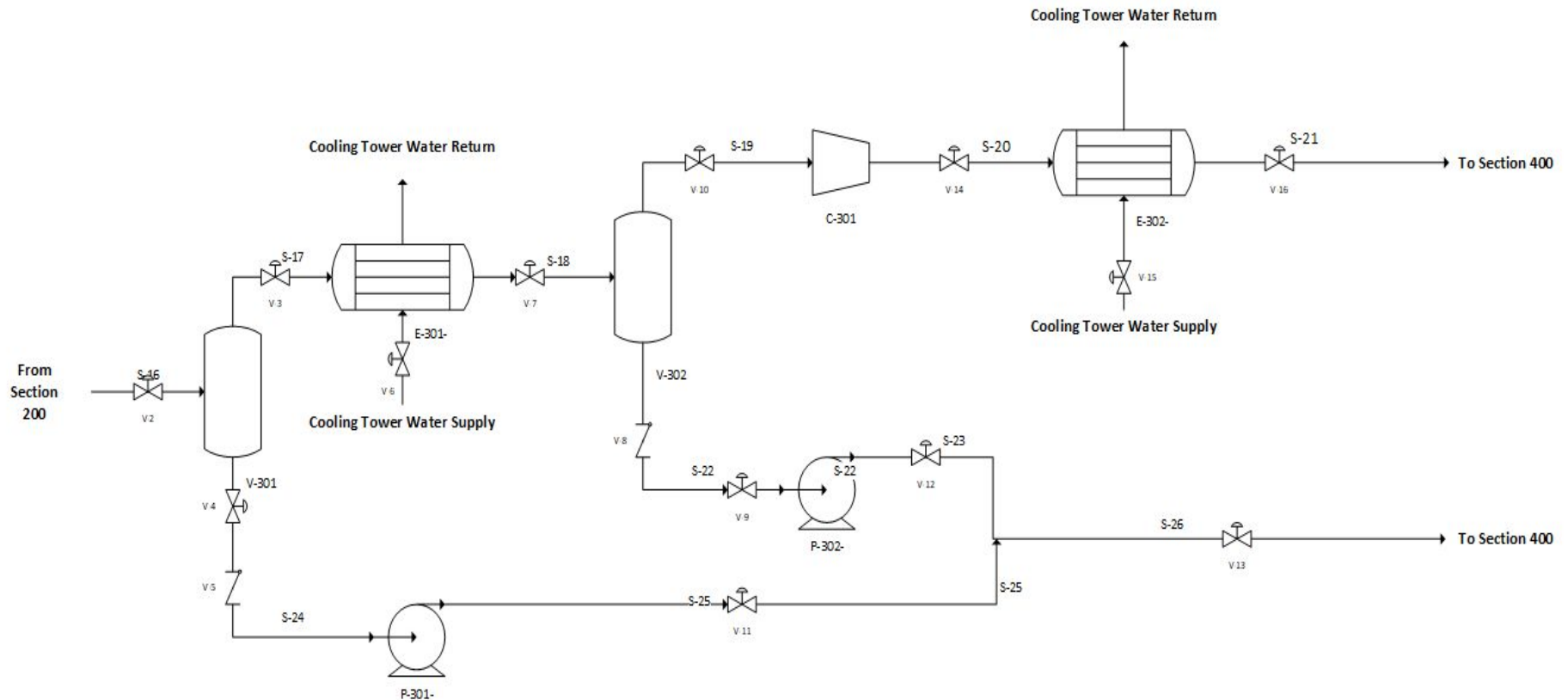
SECTION 200



SECTION 200 STREAMS

Stream	S11	S12	S13	S14	S15	S16	S400
Phase	Liquid	Liquid	Vapor	Vapor	Vapor	Mixed	Mixed
Temp. (°F)	121	150	296	662	662	231	170
Pressure (psi)	155	108	100	93	73	66	108

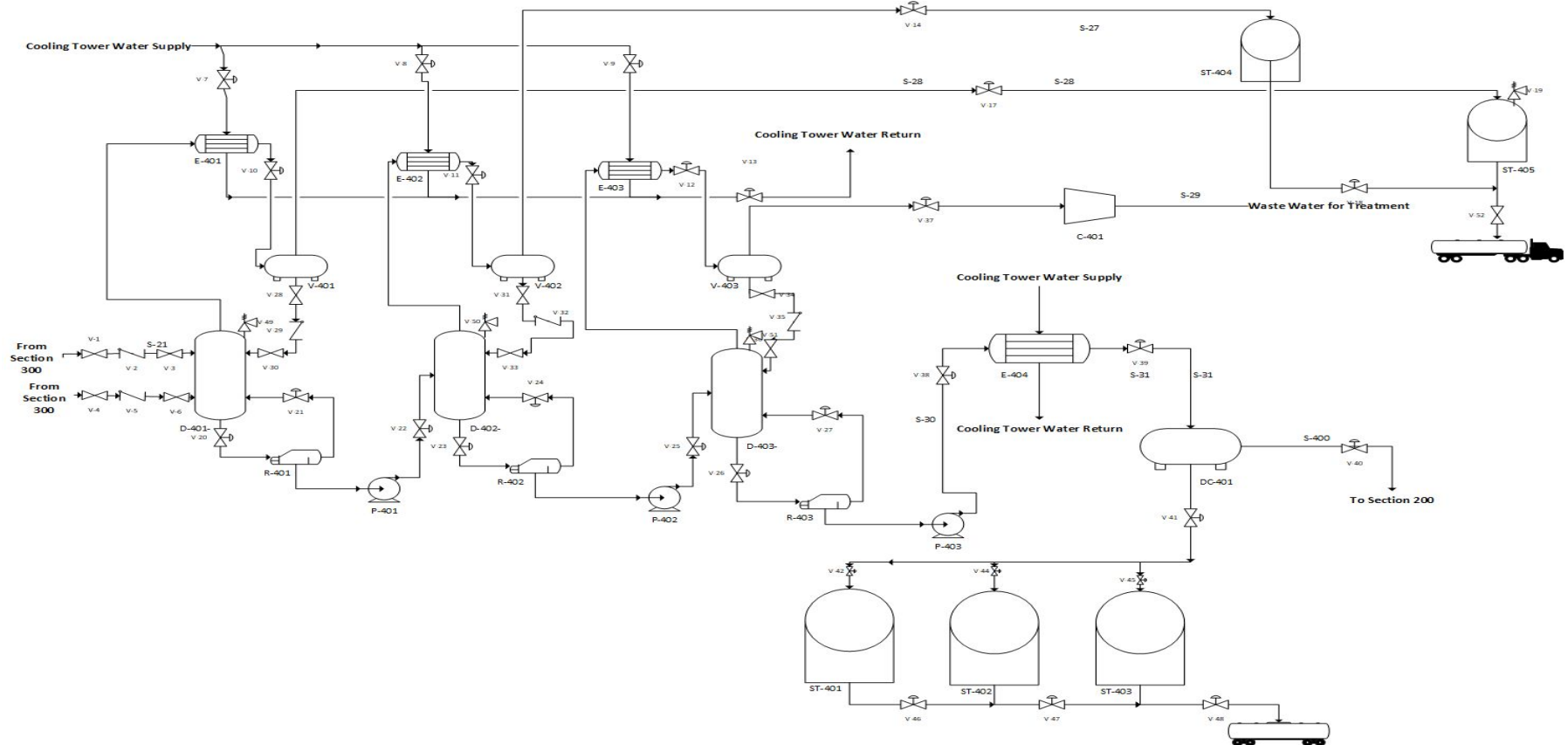
SECTION 300



SECTION 300 STREAM

Stream	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26
Phase	Mixed	Vapor	Mixed	Vapor	Vapor	Mixed	Liquid	Liquid	Liquid	Liquid	Liquid
Temp. (°F)	231	231	200	200	282	200	200	200	231	231	231
Pressure (psi)	66	66	58	58	133	126	58	125	66	125	125

SECTION 400



SECTION 400 STREAMS

Streams	S21	S26	S-27	S-28	S29	S30	S31	S400	S-33
Phase	Mixed	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°F)	200	221	108	17	110	215	170	170	110
Pressure (psi)	126	125	125	100	15	132	118	108	99

MATERIAL BALANCE

MATERIAL BALANCE FOR THE FIRST REACTOR

Shell and Tube Packed bed Reactor		
IDENTIFICATION: R-101		
FUNCTION: Dehydrogenation of ethanol into acetaldehyde and hydrogen		
OPERATION: Continuous		
MATERIALS HANDLED: (lb./hr.)	IN	OUT
Ethanol	124,340	62,170
Acetaldehyde	0	54,709
Hydrogen	0	2,486
Byproducts	0	4,973
Total	124,340	124,338
DESIGN DATA:		
Material: Stainless Steel	Catalyst Type: Copper-Chromite	
Heat source: Dowtherm	Temperature: 595°F	
Pressure : 35 psi	Residence Time: 5s	

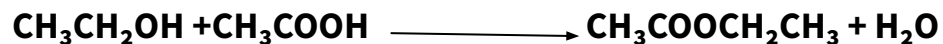
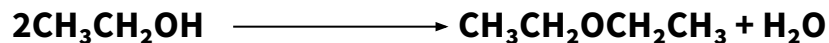
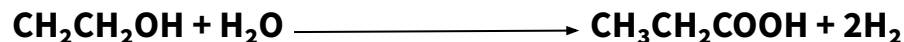
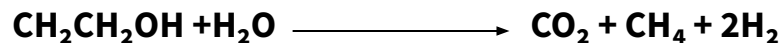
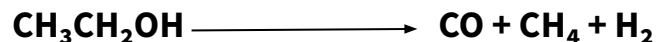
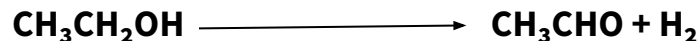
MATERIAL BALANCE FOR THE SECOND REACTOR

REACTOR		
IDENTIFICATION: R-201		
FUNCTION: To react acetaldehyde with excess ethanol to form 1,3-butadiene		
OPERATION: Continuous		
MATERIALS HANDLED: (lb./hr.)	IN	OUT
Acetaldehyde	55,676	14,524
1,3 Butadiene	0	50,505
Ethanol	110,867	67,844
Water	0	33,670
Total	166,543	166,543
DESIGN DATA:		
TYPE: <u>Fixedhead</u> , Shell-and-T		Material: Carbon Steel
Catalyst Type: 2% <u>tantala</u> , 98% silica		Temperature: 662°F
Pressure : 93 psi		Residence Time: 5s

ENERGY BALANCE

ENTHALPIES OF FORMATION

FIRST REACTION



$$\Delta H = +2,138 \text{ Btu/hr}$$

- The reaction is endothermic

❖ Carbon monoxide

❖ Methane

❖ Carbon dioxide

❖ Acetic acid

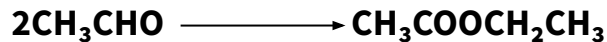
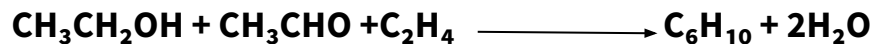
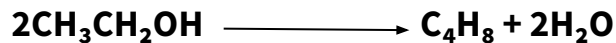
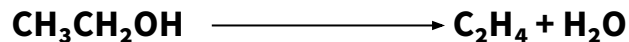
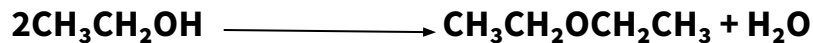
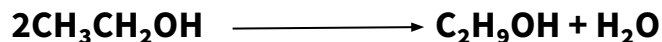
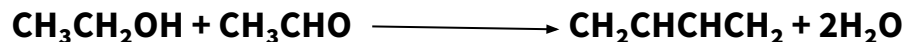
❖ Ethyl Acetate

❖ Diethyl ether

❖ Water

ENTHALPIES OF FORMATION

SECOND REACTION



$$\Delta H = +2,042 \text{ Btu/hr}$$

- ❖ Carbon monoxide
- ❖ Methane
- ❖ Carbon dioxide
- ❖ Acetic Acid
- ❖ Ethyl acetate
- ❖ Diethyl ether
- ❖ Water

EQUIPMENT ENERGY BALANCE

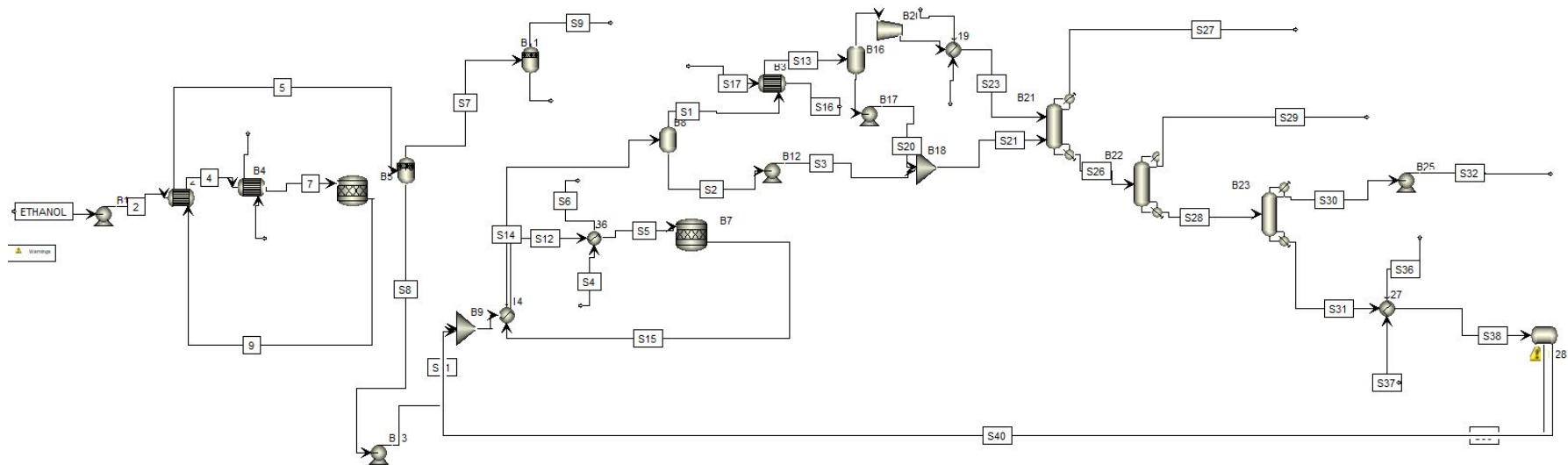
Multi-Stage Compressor	MSC-201	-60 MMBTU/hr to cool S9 from 152 °F to 107 °F	Cooling Water
Heat Exchanger	E-401	-30 MMBTU/hr to cool S28 from 231 °F to 200 °F	Cooling Water
Heat Exchanger	E-402	-20 MMBTU/hr to cool S31 from 281 °F to 200 °F	Cooling Water
Heat Exchanger	E-403	-78 MMBTU/hr to condense vapor at top of D-401 at 107 °F	Cooling Water
Heat Exchanger	E-408	-182 MMBTU/hr to condense vapor at top of D-403 at 193 °F	Cooling Water
Heat Exchanger	E-412	-83 MMBTU/hr to condense vapor at top of D-405 at 204 °F	Cooling Water
Heat Exchanger	E-414	-7 MMBTU/hr to cool S54 from 238°F to 110 °F	Cooling Water
Heat Exchanger	E-405	-3 MMBTU/hr to condense vapor at top of D2	Refrigeration
Heat Exchanger	E-410	-14 MMBTU/hr to condense vapor at top of D4	Refrigeration
Heat Exchanger	E-404	83 MMBTU/hr to boilup liquid in bottom of D-401	Steam
Heat Exchanger	E-406	5 MMBTU/hr to boilup liquid in bottom of D-402	Steam
Heat Exchanger	E-409	166 MMBTU/hr to boilup liquid in bottom of D-403	Steam
Heat Exchanger	E-411	13 MMBTU/hr to boilup liquid in bottom of D-404	Steam
Fired Heater	FH-501	100 MMBTU/hr to vaporize Dowtherm in S57 at 666 °F	Natural Gas
Fired Heater	FH-502	120 MMBTU/hr to vaporize Dowtherm in S61 at 625 °F	Natural Gas
Total Energy Requirement		110 MMBTU/hr	

R-101 Heat Duty: **46.3 MMBTU/hr** to the reactor to keep the reactor isothermal

R-201 Heat Duty: **13.6 MMBTU/hr** to the reactor to keep the reactor isothermal.

ASPEN SIMULATION

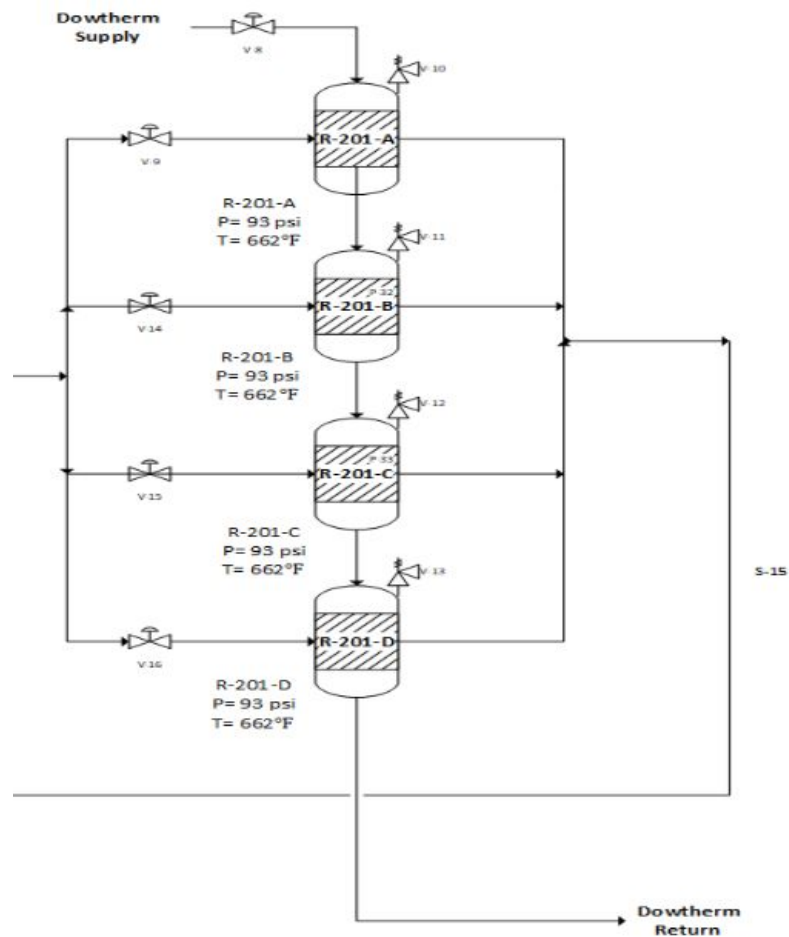
ASPEN SIMULATION



SPECIFICATION SHEET

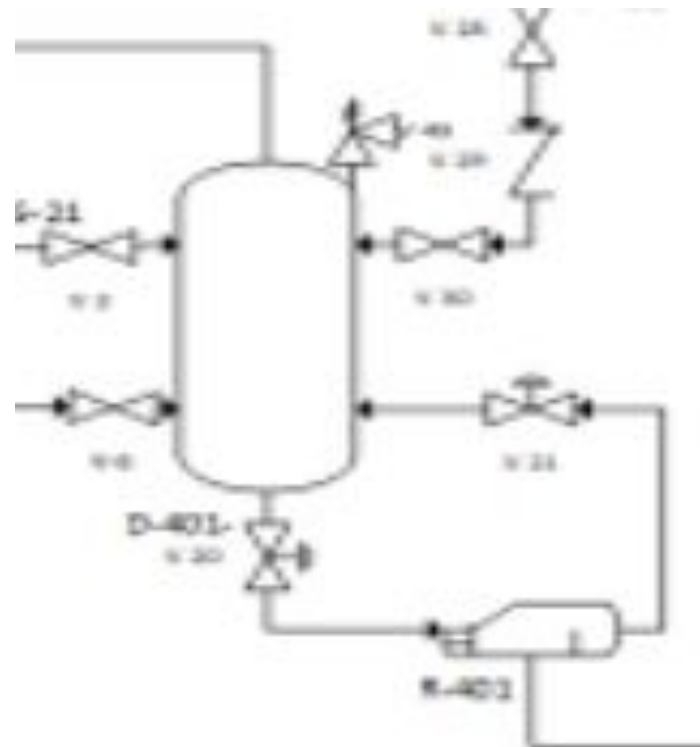
Shell and Tube Packed Bed Reactor

Identification:	Item: 4 parallel shells			
	Item No: R-201		Date: 03/10/2022	
	No. Required: 3		By:	JC
	Cost (\$)	146,000		
Function:	To react acetaldehyde with excess ethanol to form 1,3- butadiene			
Operation:	Continuous			
Materials Handled (lb/hr):	In	Out		
Acetaldehyde	66,148	17,256		
1,3 butadiene	0	57,520		
Ethanol	192,692	117,916		
Water	20,132	66,148		
Total flow (lb/hr)	287,600	287,600		
Temperature (°F)	662	662		
Pressure (psi)	93	93		
Design Data:				
Type:	Fixed Head, Shell and tube	Tube Diameter:	0.12 ft	
Material:	Carbon Steel	Tube Length:	16 ft	
Catalyst Type:	2% tantala, 98% silica	Number of Tubes:	2,747	
Catalyst Mass:	230,000 lbs.	Shell Diameter:	115 in.	
Number of shells:	4	Residence Time:	5 s	



Distillation Column

Identification:	Item:	Distillation Column		
	Item No:	D-401	Date:	
	No. Required: 1		By:	JC
	Cost (\$)	612,000		
Function:	To separate the product, butadiene, along with ethylene, from the heavy products, including ethanol, acetaldehyde, and water.			
Operation:	Continuous			
	Feed	Distillate	Bottoms	
Materials Handled:				
	274,200	60,400	213,800	
Component Flow (lb/hr):				
Ethanol	118,500	0	118,500	
Acetaldehyde	18,000	700	17,300	
Diethyl-ether	13,000	1,500	13,000	
Water	66,000	1,500	64,500	
Ethylene	2,200	2,200	0	
1,3 butadiene	56,500	56,000	500	
Temperature (°F)	220	108	280	
Pressure (psi)	126	125	129	
Tower Design Data:				
Number of Stages	37	Tray Spacing (ft)	2	
Feed Stages	12	Inside Diameter (ft)	12	
Reflux Ratio	6	Height (ft)	86	
Column Material	Carbon Steel	Tray Material	Carbon Steel	
Tower Pressure (psi)	125	Tray Type	Sieve	
Operating Temperature (°F)	Within 108-280			
Associated Components				
	Parameter	Value		
Tower				
	Equipment Type	Vertical Vessel		
	Weight (lbs.)	165,000		
	Thickness (in)	2.5		
	Bare Module Cost			
Condenser				
	Equipment Type	Fixed Head Heat Exchanger		
	Heat Duty	.78 MMBTU/ hr		
	Shell Material	Carbon Steel		



SAFETY & HANDLING

SAFETY

- ❑ 1,3 Butadiene is extremely flammable
- ❑ May cause explosive mixture with air
- ❑ May cause frostbite
- ❑ Contains gas under pressure; may explode if heated
- ❑ Inhalation may cause cancer and genetic defects

Butadiene



Colorless, gas; mild aromatic odor. Irritating to eyes/respiratory tract. Skin contact may cause frostbite. Also causes: drowsiness, possible reproductive/teratogenic effects (based on animal data). Suspect cancer hazard. Explosive. Flammable.

CAS No. 106-99-0

! DANGER



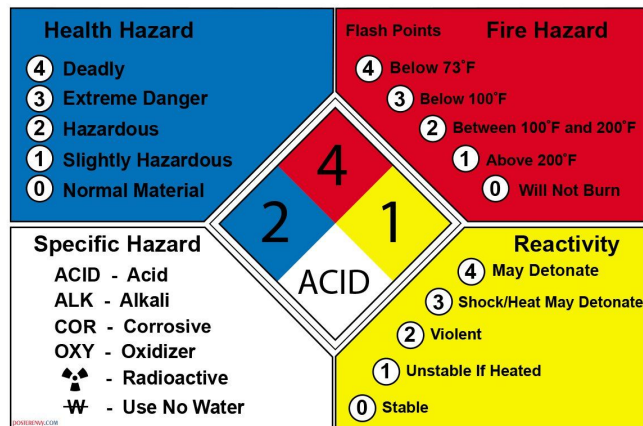
Butadiene

SAFETY (Hydrogen)

- ❑ Hydrogen has a wide flammability range, and can form an explosive mixture with air.
- ❑ Hydrogen can be explosive at concentrations of 18.3%-59%.
- ❑ Gaseous hydrogen cannot be detected by the human senses, and its flame is also invisible.
- ❑ Hydrogen diffuses through materials not normally considered porous.
- ❑ Handling liquid hydrogen can bring evaporation problems that require adopting certain measures.
- ❑ Leaks have to be controlled.
- ❑ Due to its small size, hydrogen can cause embrittlement of high strength steels, titanium and aluminum alloys, with cracking and catastrophic failure of the metals.
- ❑ Hydrogen requires only a small amount of energy for ignition (0.02 mJ)

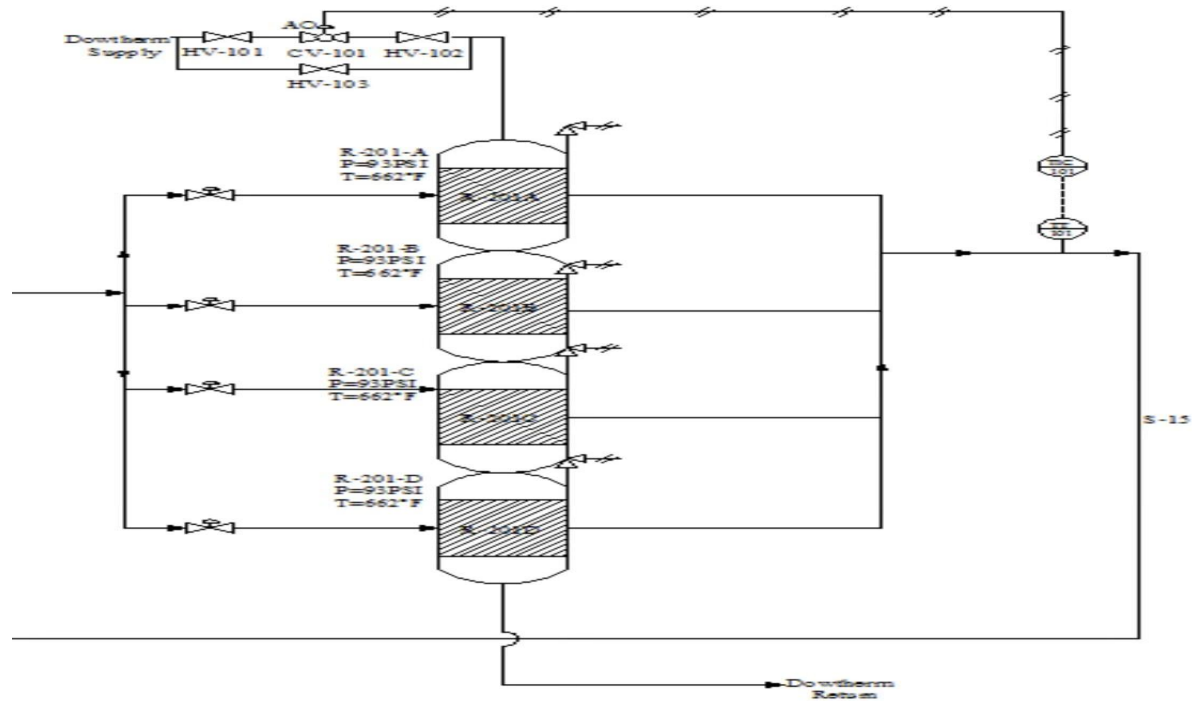
HANDLING

- ❑ Obtain special instructions before use
- ❑ Do NOT handle chemical until safety precautions have been read and understood
- ❑ Keep away from heat, open flames, sparks, hot surfaces
- ❑ Avoid breathing gas
- ❑ Use and store only outdoors or in well-ventilated area
- ❑ Wear your PPE like protective gloves, protective clothing, eye protection, respiratory protection and/or face protection



	Fire Hazard (Flammability)	Health Hazard	Reactivity (Instability)
Rating	Description of Numeric Rating		
4	Flash Point < 73°F Boiling Point < 100°F	Deadly	May detonate
3	Flash Point < 73°F and Boiling Point ≥ 100°F, or Flash Point 73°F to 100°F	Extreme danger	Shock and heat may detonate
2	Boiling Point > 100°F and ≤ 100°F	Hazardous	Violent chemical change
1	Flash Point > 200°F	Slightly hazardous	Unstable if heated
0	Will not burn	Normal material	Stable

P&ID for R-201



EQUIPMENT SAFETY (HAZOP)

Process parameter	Deviation	Possible consequences	Possible causes	Action required/ Safeguards
Pressure	More	- High/rising velocity of reactant - Overpressure of the process - High/rising temperature	- Valve failure - Overheating of the column/separator	- Installation of High pressure/ High temperature alarm - Installation of safety valve
	Less	- Less reaction - Less favorable product	- Leakage in the process - Compressor failure	- Insertion of safety valve - Installation of low pressure alarm
Temperature	More	- Uncontrolled reaction - Mechanical failure - May cause explosion	- Pressure/temperature instrument failure - Too much heat supplied from the heat source - Fan failure	Installation of temperature/pressure sensor
	Less	Less pressure, less favorable product.	Too little heat supplied from the heat source	Installation of temperature/pressure sensor
Ignition	-	- Fire, sparks - Runaway reactions - Explosion	- Presence of oxidizing substance - Temperature rise	- Insulation of piping and equipment - Temperature sensor

EQUIPMENT SAFETY CONSIDERATIONS

- ❑ Reactors: endothermic catalytic reaction
 - ❑ Hazards: Thermal runaway
 - ❑ Solutions: Both reactors run at high temperature: stainless steel material must be considered, and use of special process heaters, Using the safeguards against any unpredict over heat generation release.
- ❑ Distillation: simple distillation
 - ❑ Hazards: Involve large quantities of potential energy in the form of utility energy or associated in the process , process so sensitive to even the little change
 - ❑ under pressure vacuum concern and the loss of heat input to a distillation result in rapid collapse of vapor at the top of the column
 - ❑ Solutions: alarm system for too high or too low changing
 - ❑ Estimate risk and likelihood to happen before designing
 - ❑ Estimate designing to accommodate full vacuum
- ❑ Pumps/ Compressors and Heat Exchangers
 - ❑ Hazards: failure, cavitation
 - ❑ Solution(s): Standby pumps
- ❑ In general any manufacturing system need safeguards and pressure ,vacuum relief system alarms , fixed fire protection , Passive mitigation and system wide concern

FUTURE WORK

WHAT COULD WE DO TO IMPROVE THE PLANT?

- Possibly add more Distillation Column
- Insure of a safety procedure for plant protocol
- Instruct plan for saving energy on plant
- Order a cost effective design
- Find a way to reduce the overall investment

CONCLUSION

- Ethanol is a feedstock of manufacturing 1,3 butadiene by non-oxidative dehydrogenation of ethanol forming hydrogen and acetaldehyde.
- Acetaldehyde is a main product of ethanol conversion which involved in subsequent reaction steps led to 1,3- butadiene.
- Our product is essential in manufacturing world necessities.
- Expect estimation of producing 1,3 BD will reach to 19.6 million tons by 2027. based on data bridge market research because of the high demand of butadiene for consumer product on the other hand not to forget the role of ethanol itself globally.
- Important to shed light on health concern studies and risk researches about 1,3 BD.
- Many country producing the 1,3 Butadiene due the high demand on it , like North America , Canada , Asia , Latin America and Middle East .

REFERENCES

- ❑ Bradley, Jean-Claude. "UPenn Library Open Notebook Science Talk Jan 2010." SciVee (n.d.): n. pag. Web. Corson, B. B., et al.
- ❑ "Ethanol Producer Magazine – The Latest News and Data About Ethanol Production." *Ethanol Producer Magazine – The Latest News and Data About Ethanol Production*. N.p., n.d. Web. 8 Nov. 2016.
- ❑ Stahly, E. E., et al., "Butadiene from Ethanol," Ind. Eng. Chem., 40, 12, 2301-2303 (1948).
- ❑ "ChemInform Abstract: Review of Old Chemistry and New ..." N.p., n.d. Web. 10 Nov. 2016.
- ❑ "Renewable Fuels Association." Renewable Fuels Association. N.p., n.d. Web. 7 Nov. 2016.

THANK YOU!!!

(Questions, Comments, Concerns?)

APPENDIX

MARKET ANALYSIS

- ❑ Global 1,3 butadiene market analysis was 23148556.412 pound in 2013
- ❑ Asia pacific emerged as the largest regional market for BD for 53.6% market volume in 2013
- ❑ China recognize as the largest manufacturer of 1,3 BD through the naphtha cracking process
- ❑ BD market in Europe and North America is characterised by growing demand
- ❑ North America reached to 30% of global share due to consuming of it through the industrial manufacturing
- ❑ Europe has steady growth of demand 1,3 BD
- ❑ Middle East and Latin America account for merely single digits share in global 1,3 butadiene market

SAFETY PROCESS

The health effects caused by exposure to 1,3-butadiene can be under two categories

- Acute exposure
- Chronic effect

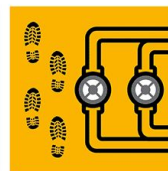
1,3 butadiene is on Hazardous substance

that is cited by:

- OSHA (Occupational Safety and Health Association)
- ACGIH
- DOT
- NIOSH
- NTP
- DEP
- EPA and NFPA



Maintain safe isolation



Walk the line



Apply procedures



Sustain barriers



Control ignition sources



Recognize change



Respect hazards



Stay within operating limits



Stop if the unexpected occurs



Watch for weak signals

EQUIPMENT NAMES

Equipment	Description
ST 101	Storage Tank
P 101	Pump
E 101	Heat Exchanger
E 102	Heat Exchanger
R 101	Reactor
V 101	Pressurized Vessel
PSA 101	Pressure swing absorbed
E 201	Heat Exchanger
E 202	Heat Exchanger
R 201	Reactor Two

Equipment	Description
C-301	Centrifugal Compressor
E-301	Shell-and-tube heat Exchanger
E-302	Shell-and-tube Heat Exchanger
P-301	Centrifugal Pump
P-302	Centrifugal Pump
V-301	Vertical Pressurized Vessel
V-302	Vertical Pressurized Vessel

EQUIPMENT NAMES CONTINUED....

Equipment	Description
B-401	Kettle Reboiler
B-402	Kettle Reboiler
B-403	Kettle Reboiler
C-401	Centrifugal Compressor
D-401	Distillation Tower
D-402	Distillation Tower
D-403	Distillation Tower
DC-401	Decanter
E-401	Shell-and-Tube Heat Exchanger

Equipment	Description
E-402	Shell- and-Tube Heat Exchanger
E-403	Shell- and-Tube Heat Exchanger
E-404	Shell- and-Tube Heat Exchanger
P-401	Centrifugal Pump
P-402	Centrifugal Pump
P-403	Centrifugal Pump
ST-401	Spherical Pressurized
ST-402	Spherical Pressurized
ST-403	Vertical Pressurized
ST-404	Vertical Pressurized

Relevant Calculations for R-101 & R-201

- Volume of Ethanol: $V_{ethanol} = \frac{n_{ethanol} \cdot MW}{\rho_{ethanol}}$
- Tube Bundle Internal Volume Calculation: $V = \pi \cdot (tube\ inner\ radius)^2 \cdot L_{tube}$
- Number of tubes: $N_t = \frac{total\ volumetric\ flowrate}{volumetric\ flowrate_{one\ tube}}$, with

$$\bullet\ Volumetric\ flowrate_{one\ tube} = \frac{tube\ volume}{contact\ time}$$

- Superficial velocity through a tube: $V_{one\ tube} = \frac{Volumetric\ flowrate_{one\ tube}}{cross\ sectional\ area\ of\ one\ tube}$
- Volume of catalyst: $V_{catalyst} = N_t * Volumetric\ flowrate_{one\ tube}$
- Tube side pressure drop:

$$\Delta P = \frac{150 * \mu_{fluid} * (1-\epsilon)^2 * L_{tube}}{\phi_S^2 * D_p * \epsilon^3} * V_{superficial} + \frac{1.75 * \mu_{fluid} * (1-\epsilon)^2 * L_{tube}}{\phi_S^2 * D_p * \epsilon^3} * (V_{superficial})^2$$

- Shell Diameter: $D_S = \sqrt{\left(\frac{N_t}{3} * (square\ pitch)^2 * \frac{4}{\pi}\right)} + 2 * tube\ outer\ diameter + 1$
- Heat transfer coefficient: $U = \frac{Q}{A * \Delta T}$

Shell and Tube Packed Bed Reactor				
Identification:	Item: 4 parallel shells			
	Item No: R-101		Date: 03/10/2022	
	No. Required: 3		By:	JC
	Cost (\$):	183,000		
Function:	Dehydrogenation of ethanol into acetaldehyde and hydrogen gas			
Operation:	Continuous			
Materials Handled (lb/hr):	In	Out		
Ethanol	148,000	76,616		
Acetaldehyde	0	65,000		
Hydrogen	0	3,100		
Water	7,800	7,700		
Acetic Acid	0	535		
Ethyl Acetate	0	1,100		
Methane	0	200		
Carbon Dioxide	0	300		
Diethyl Ether	0	780		
Total Flow (lb/hr)	155,000	155,000		
Temperature (°F)	595	595		
Pressure (psi)	35	35		
Design Data:				
Type:	Floating Head, Shell and Tube			
Material:	Stainless Steel	Tube Length	20 ft	
Catalyst Type:	Copper- Chromite	Tube Diameter	0.125ft	
Catalyst Mass:	907,000 lbs	Number of Tubes	2750 per shell	
Number of Shells:	4	Residence Time:	5 s	
Heat Source	DowTherm	Utility (lb/hr):	407,000	

Distillation Column				
Identification:	Item:	Distillation Column		
	Item No:	D-401	Date:	
	No. Required: 1		By:	JC
	Cost (\$)	612,000		
Function:	To separate the product, butadiene, along with ethylene, from the heavy products, including ethanol, acetaldehyde, and water.			
Operation:	Continuous			
	Feed	Distillate	Bottoms	
Materials Handled:				
	274,200	60,400	213,800	
Component Flow (lb/hr):				
Ethanol	118,500	0	118,500	
Acetaldehyde	18,000	700	17,300	
Diethyl-ether	13,000	1,500	13,000	
Water	66,000	1,500	64,500	
Ethylene	2,200	2,200	0	
1,3 butadiene	56,500	56,000	500	
Temperature (°F)	220	108	280	
Pressure (psi)	126	125	129	
Tower Design Data:				
Number of Stages	37	Tray Spacing (ft)	2	
Feed Stages	12	Inside Diameter (ft)	12	
Reflux Ratio	6	Height (ft)	86	
Column Material	Carbon Steel	Tray Material	Carbon Steel	
Tower Pressure (psi)	125	Tray Type	Sieve	
Operating Temperature (°F)	Within 108-280			
Associated Components				
	Parameter	Value		
Tower				
	Equipment Type	Vertical Vessel		
	Weight (lbs.)	165,000		
	Thickness (in)	2.5		
	Bare Module Cost			
Condenser				
	Equipment Type	Fixed Head Heat Exchanger		
	Heat Duty	.78 MMBTU/ hr		
	Shell Material	Carbon Steel		

EQUIPMENT	DESCRIPTION	Cp (cost of purchase, USD22)	EQUIPMENT PURCHASE COST
ST 101	Storage Tank	1,000,000	
P 101	Pump	24,400	
E 101	Heat Exchanger	135,000	
E 102	Heat Exchanger	667,000	
R 101	Reactor	183,000	
V 101	Pressurized Vessel	25,900	
PSA 101	Pressure swing adsorber	5,366,000	
E 201	Heat Exchanger	148,000	
E 202	Heat Exchanger	749,000	
R 201	Reactor	146,000	
	Sections 100 & 200 Cp Total (USD)	8,444,300	

EQUIPMENT PURCHASE COST

EQUIPMENT	DESCRIPTION	Cp (Cost of purchase, USD22)
C 301	Centrifugal Compressor	1,030,000
E 301	Heat Exchanger	100,000
E 302	Heat Exchanger	79,000
P 301	Pump	9,825
P 302	Pump	8,123
V 301	Vertical Pressurized Vessel	25,400
V 302	Vertical Pressurized Vessel	17,900
	Section 300 Cp Total (USD)	1,270,248

EQUIPMENT PURCHASE COST

EQUIPMENT	DESCRIPTION	Cp (cost of purchase, USD)
B 401	Kettle Reboiler	312,000
B 402	Kettle Reboiler	18,340
B 403	Kettle Reboiler	316,000
C 401	Centrifugal Compressor	1,349,300
D 401	Distillation Tower	612,000
D 402	Distillation Tower	447,000
D 403	Distillation Tower	583,000
DC 401	Decanter	31,500
E 401	Heat Exchanger	1,169,000
E 402	Heat Exchanger	86,500
E 403	Heat Exchanger	272,000
E 404	Heat Exchanger	36,500
P 401	Centrifugal Pump	25,000
P 402	Centrifugal Pump	22,000
P 403	Centrifugal Pump	10,000
ST 401	Special Pressurized Tank	593,500
ST 402	Special Pressurized Tank	232,000
ST 403	Vertical Pressurized Tank	593,500
ST 404	Vertical Pressurized Tank	593,500
	Section 400 Cp Total (USD)	5,953,340

ESTIMATION OF CAPITAL INVESTMENT BY PERCENTAGE OF DELIVERED EQUIPMENT

(See Table 6-9)

The fractions in the cells below are approximations applicable to typical plants. These values may differ depending on many factors such as location,

Required user input	Default		Subtotal	Result
Required, from a linked sheet or				Notes & comments

Project Identifier: Illustration 101	Fraction of delivered equipment			User: Calculated values, million \$
	Solid-processin g plant	Solid-fluid processin g plant	Fluid processin g plant	copy from values at left or

Direct Costs				
Purchased equipment, E'				24,000
Delivery, fraction of E'	0.10	0.10	0.10	2,400
Subtotal: delivered				26,400
Purchased equipment	0.45	0.39	0.47	12,408
Instrumentation&Controls(ins	0.18	0.26	0.36	9,504
Piping (installed)	0.16	0.31	0.68	17,952
Electrical systems (installed)	0.10	0.10	0.11	2,904
Buildings (including services)	0.25	0.29	0.18	4,752
Yard improvements	0.15	0.12	0.10	2,640
Service facilities (installed)	0.40	0.55	0.70	18,480
Total direct costs	1.69	2.02	2.60	35,040

Indirect Costs				
Engineering and supervision	0.33	0.32	0.33	8,712
Construction expenses	0.39	0.34	0.41	10,824
Legal expenses	0.04	0.04	0.04	1,056
Contractor's fee	0.17	0.19	0.22	5,808
Contingency	0.35	0.37	0.44	11,616
Total indirect costs	1.28	1.26	1.44	38,016

Fixed capital investment (FCI)				133,056
---------------------------------------	--	--	--	---------

Working capital	0.70	0.75	0.89	0.89	23,496
------------------------	------	------	------	------	--------

Total capital investment (TCI)					156,552
---------------------------------------	--	--	--	--	---------

The investments are made over a period of time. This is represented on the basis that startup (time 0) will be three years after the date of the estimate, that 15% of the fixed capital investment is spent in the year beginning at the time of the estimate (year ending at time -2), 35% in the second year ending at -1, and 50% in the third year ending at time 0). These values may be

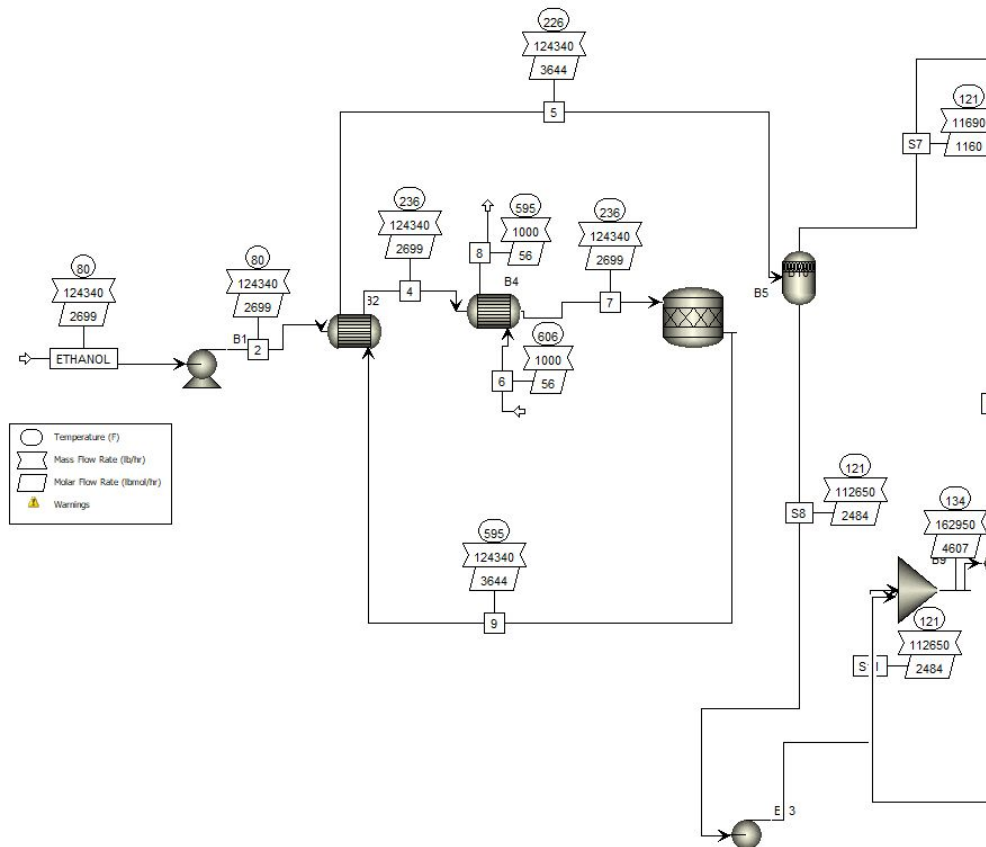
Scale "Estimation" and
"Year-0 \$", then
adjusted as described below

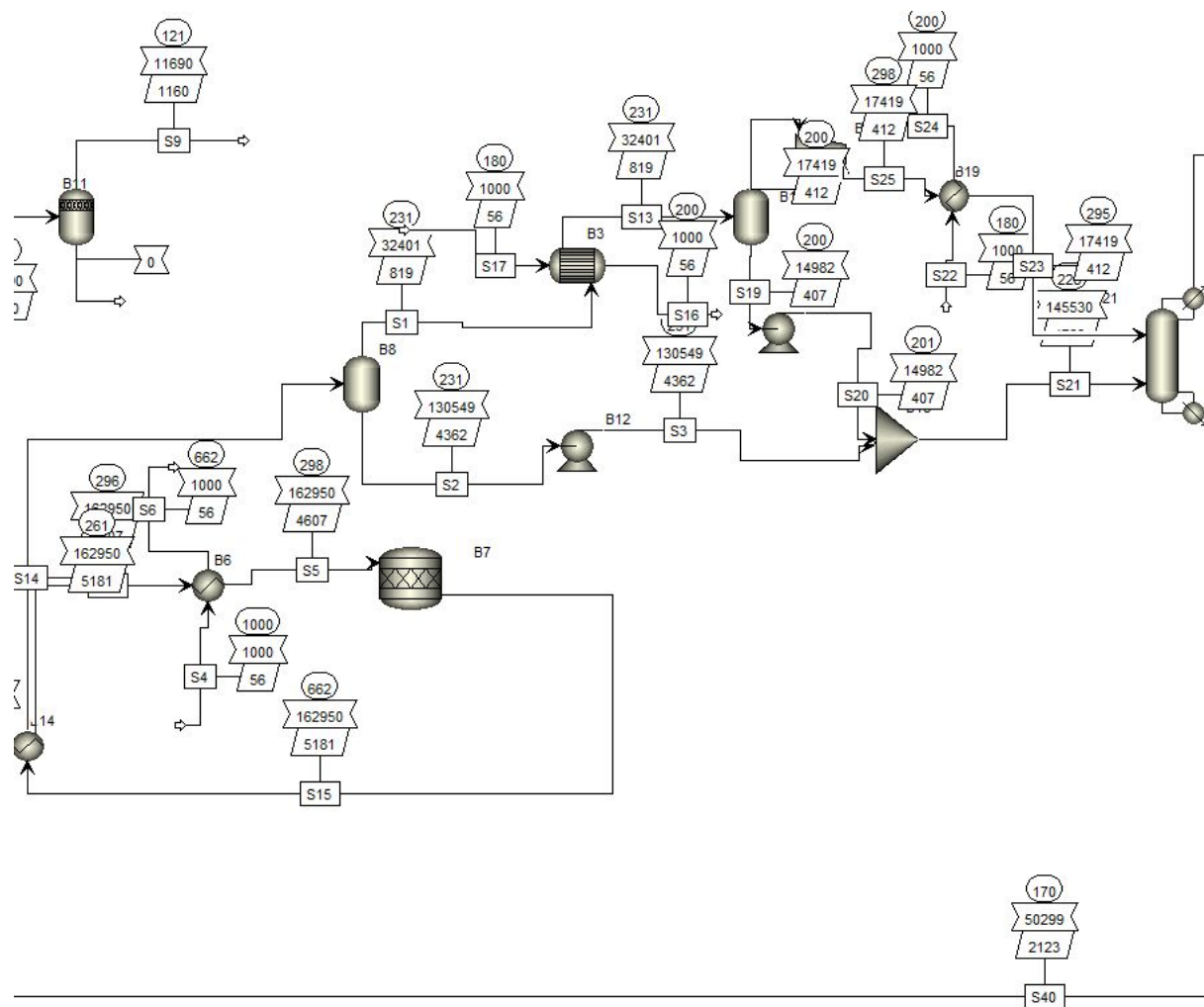
RESULT			
Products, Coproducts and Byproducts			
Name of Material	Price, \$/kg	Annual Amount, million kg/y	Annual value of product, million \$/y
1,3 BD	2.20	182.000	400.40
H2	3.25	10.700	34.78
			0.00
			0.00
			0.00
			0.00
Total annual value of products =			435.18
			Sent to 'Evaluation' and 'Year-0 \$'

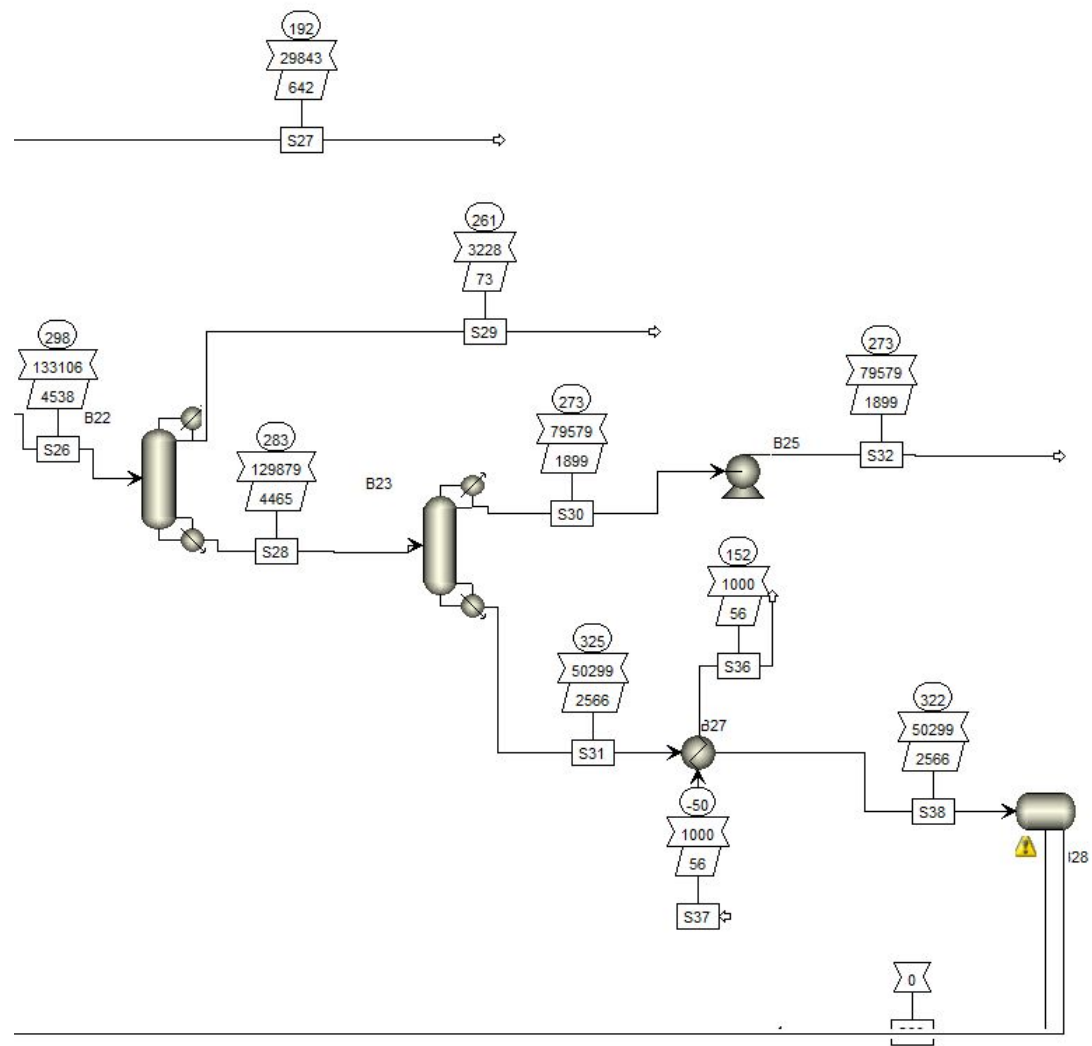
Raw Materials			
Name of Material	Price, \$/kg	Annual Amount, million kg/y	Annual raw materials cost,
1	0.73	525.000	383.25
			0.00
			0.00
			0.00
Total annual cost of raw materials =			383.25
			Sent to sheet

RESULT			
Operating Labor			
Number of operators per shift*	Shifts per day**	Operator rate, \$/h #	Annual operating labor cost,
8	3	33.67	2.360
*See Tables 6-13 and Fig. 6-9.			
**Default = 3 for continuous process.			
Enter appropriate value for batch operation.			
#To obtain current, local value, enter (latest local ENR skilled labor index)/6067 =			
			1

Sent to sheet 'Annual TPC'					
Utility	Default unit cost	Default cost units	Annual utility requirement, in appropriate units	Default units of utility requirement	Annual utility cost, million \$/y
Air, compressed					
Process air	0.45	\$/100m ³ #	2000000	100 m ³ /y	0.900
Instrument air	0.90	\$/100m ³ #	3000000	100 m ³ /y	2.700
Electricity					
Purchased, U.S. average	0.045	\$/kWh		kWh/y	2.500
Self-generated	0.05	\$/kWh		kWh/y	0.000
Fuel					
Coal	1.66	\$/GJ		GJ/y	0.000
Fuel oil	3.30	\$/GJ		GJ/y	0.000
Natural gas	3.00	\$/GJ	360000	GJ/y	1.080
Manufactured gas	12.00	\$/GJ	2000000	GJ/y	24.000
Refrigeration, to temperature					
15 °C	4.00	\$/GJ		GJ/y	0.000
5 °C	5.00	\$/GJ		GJ/y	0.000
-20 °C	8.00	\$/GJ		GJ/y	0.000
-50 °C	14.00	\$/GJ		GJ/y	0.000
Steam, saturated					
3550 kPa	8.00	\$/1000 kg		1000 kg/y	0.000
790 kPa	6.00	\$/1000 kg	40000	1000 kg/y	0.240
Exhaust (150 kPa)	2.00	\$/1000 kg		1000 kg/y	0.000
Waste water					
Disposal	0.53	\$/m ³		m ³ /y	
Treatment	0.53	\$/m ³	31000000	m ³ /y	16.430
Waste disposal					
Hazardous	145.00	\$/1000 kg		1000 kg/y	0.000
Non-hazardous	36.00	\$/1000 kg		1000 kg/y	0.000
Water					
Cooling	0.08	\$/m ³	15000000	m ³ /y	1.200
Process					
General	0.53	\$/m ³	400000	m ³ /y	0.212
Distilled	0.90	\$/m ³		m ³ /y	0.000
# measured at 101.3 kPa and 15°C.					









	Units	2	3	4	5	6	7	8	9	ETHANOL	
► Description											
► From		B1	B9	B2	B2		B4	B4	B5		
► To		B2	B14	B4	B10	B4	B5		B2	B1	
► Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	
► Maximum Relative Error											
► Cost Flow	\$/hr										
► - MIXED Substream											
► Phase		Liquid Phase	Liquid Phase		Vapor Phase	Vapor Phase		Vapor Phase	Vapor Phase	Liquid Phase	
► Temperature	F	80.3101	133.829	235.54	226	606	235.54	595	595	80	
► Pressure	psia	50	108	50	35	50	50	50	35	15	
► Molar Vapor Fraction		0	0	0.204062	1	1	0.204188	1	1	0	
► Molar Liquid Fraction		1	1	0.795938	0	0	0.795812	0	0	1	
► Molar Solid Fraction		0	0	0	0	0	0	0	0	0	
► Mass Vapor Fraction		0	0	0.204062	1	1	0.204188	1	1	0	
► Mass Liquid Fraction		1	1	0.795938	0	0	0.795812	0	2.2505e-10	1	
► Mass Solid Fraction		0	0	0	0	0	0	0	0	0	
► Molar Enthalpy	Btu/lbmol	-119213	-109751	-110681	-67084.5	-99573.2	-110679	-99668.3	-60764.1	-119222	
► Mass Enthalpy	Btu/lb	-2587.71	-3102.79	-2402.5	-1965.83	-5527.15	-2402.45	-5532.43	-1780.62	-2587.9	
► Molar Entropy	Btu/lbmol-R	-82.6126	-56.7629	-69.5824	-28.4676	-7.37544	-69.5796	-7.46518	-21.1619	-82.6292	
► Mass Entropy	Btu/lb-R	-1.79323	-1.60476	-1.51039	-0.83421	-0.409399	-1.51033	-0.41438	-0.620126	-1.79359	
► Molar Density	lbmol/cuft	1.07918	1.38111	0.0319441	0.0047566	0.00437211	0.0319251	0.00441771	0.00309239	1.07945	
► Mass Density	lb/cuft	49.7166	48.8519	1.47163	0.16232	0.0787647	1.47076	0.0795862	0.105529	49.7291	
► Enthalpy Flow	Btu/hr	-3.21756e+08	-5.05599e+08	-2.98727e+08	-2.44432e+08	-5.52715e+06	-2.98721e+08	-5.53243e+06	-2.21402e+08	-3.2178e+08	
► Average MW		46.069	35.3716	46.069	34.1252	18.0153	46.069	18.0153	34.1252	46.069	
► ✦ Mole Flows	lbmol/hr	2698.99	4606.8	2698.99	3643.64	55.5084	2698.99	55.5084	3643.64	2698.99	
► ✦ Mole Fractions											
► ✦ Mass Flows	lb/hr	124340	162950	124340	124340	1000	124340	1000	124340	124340	
► ✦ Mass Fractions											
► Volume Flow	cuft/hr	2500.97	3335.58	84491.1	766018	12696	84541.3	12565	1.17826e+06	2500.35	
► ✦ Vapor Phase											
► ✦ Liquid Phase											

BELOW AVERAGE

**Below Average Student Original Graded Assignment on Final Project
Powerpoint Presentation**



Chem-OI

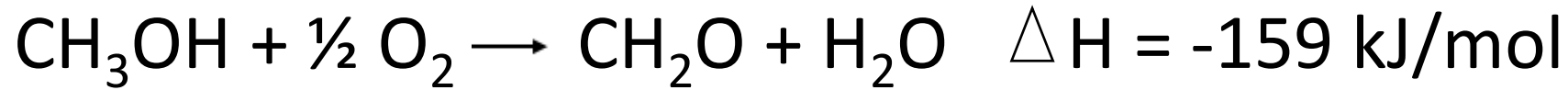
Dada Team 5: Abdul-Rahman Zakir, Alessia Williams, Nathan Warren, Timothy Waugh, Xavier Williamson

76% 89% 83% 63% 74%

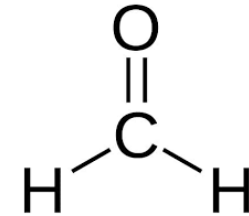
Task	Duration	Start Date	End Date
1) REVIEW & MODIFY	8	1/21/2022	1/29/2022
1.1 Update PFD	8	1/21/2022	1/29/2022
1.2 Regulations	8	1/21/2022	1/29/2022
1.3 Material Balance	8	1/21/2022	1/29/2022
2) SIMULATION	60	2/1/2022	4/1/2022
2.1: Heat Exchangers	30	2/1/2022	3/3/2022
2.2 : Reator	30	3/3/2022	4/1/2022
2.3: Absorption Column	30	3/3/2022	4/1/2022
3) DESIGN	60	2/1/2022	4/1/2022
3.1: Air Feed Heat Exchanger	60	2/1/2022	4/1/2022
3.2: Methanol Vaporizer	60	2/1/2022	4/1/2022
3.3: Reactor	60	2/1/2022	4/1/2022
3.4: Product Stream Heat Exchanger	60	2/1/2022	4/1/2022
3.5: Absorption Column	60	2/1/2022	4/1/2022
4) PIPING & INSTRUMENTATION DESIGN	8	4/1/2022	4/8/2022
4.1 : Sensor Placement	8	4/1/2022	4/8/2022
4.2: Control Valve Placement	8	4/1/2022	4/8/2022
4.3: Waste Management & Storage Placement	8	4/1/2022	4/8/2022
5): ECONOMIC ANALYSIS	15	4/1/2022	4/15/2022
5.1: CapCost	15	4/1/2022	4/15/2022
5.2: Present Value Ratio	15	4/1/2022	4/15/2022
5.3: Net Present Value	15	4/1/2022	4/15/2022
5.4: Payback Period	15	4/1/2022	4/15/2022
6) REPORT & PRESENTATION SYNTHESIS	9	4/15/2022	4/23/2022
6.1 : Synthesize PFD & P&ID	5	4/15/2022	4/19/2022
6.2: Synthesize Waste Management	5	4/15/2022	4/19/2022
6.3: Synthesize Economic Analysis	5	4/15/2022	4/19/2022

Project Schedule

Introduction

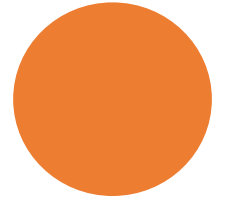


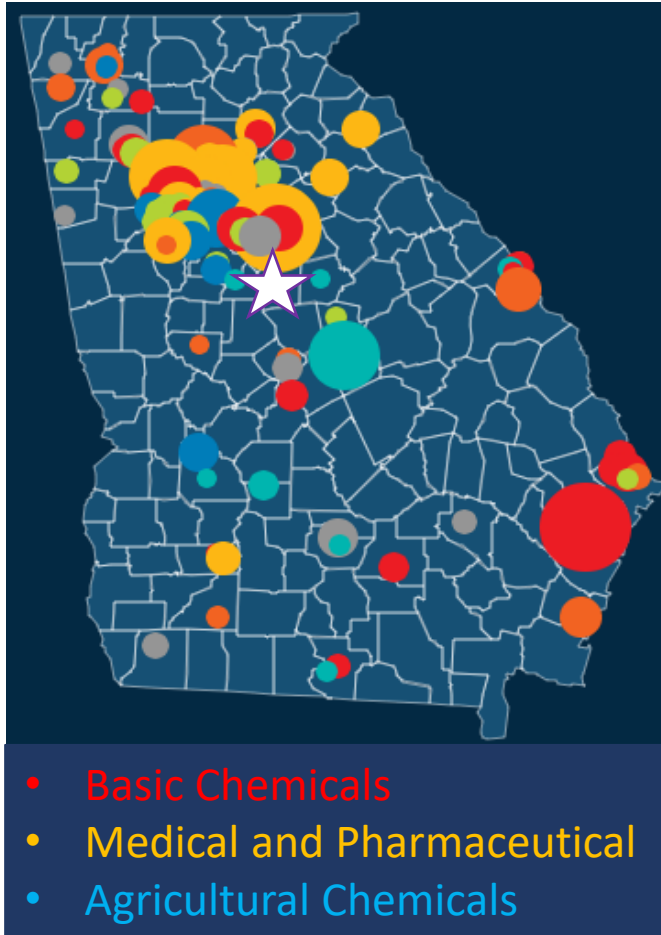
- Product: Formalin- 55 wt% aqueous solution of formaldehyde
- Uses: Resins, antiseptics, fertilizers, etc.
- Plant Location: Monticello, Georgia
- Process: Metal oxide catalyst (Iron-Molybdenum) - exothermic, high conversion, pure products



Plant Location

- **Location** - Monticello, Georgia
- No extensive emission regulations
- Access to raw materials for production
- Access to water from Jackson Lake





Plant Location

Customers:

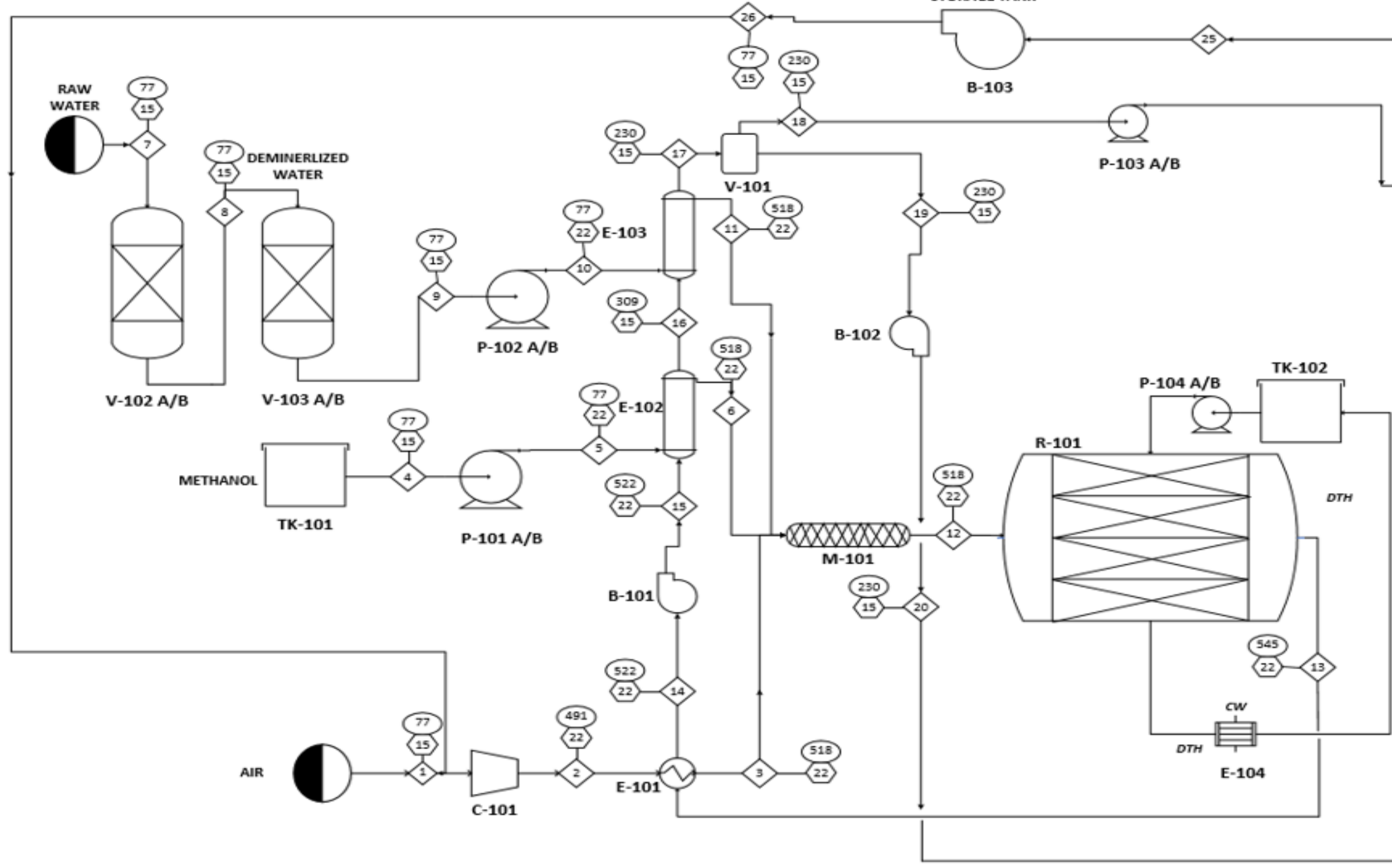
- Canal Wood LLC (Monticello, 40% sales)
- Dow Chemical Company (Marietta, 35% sales)
- BASF (Middle, 20 % sales)

Competition in vicinity:

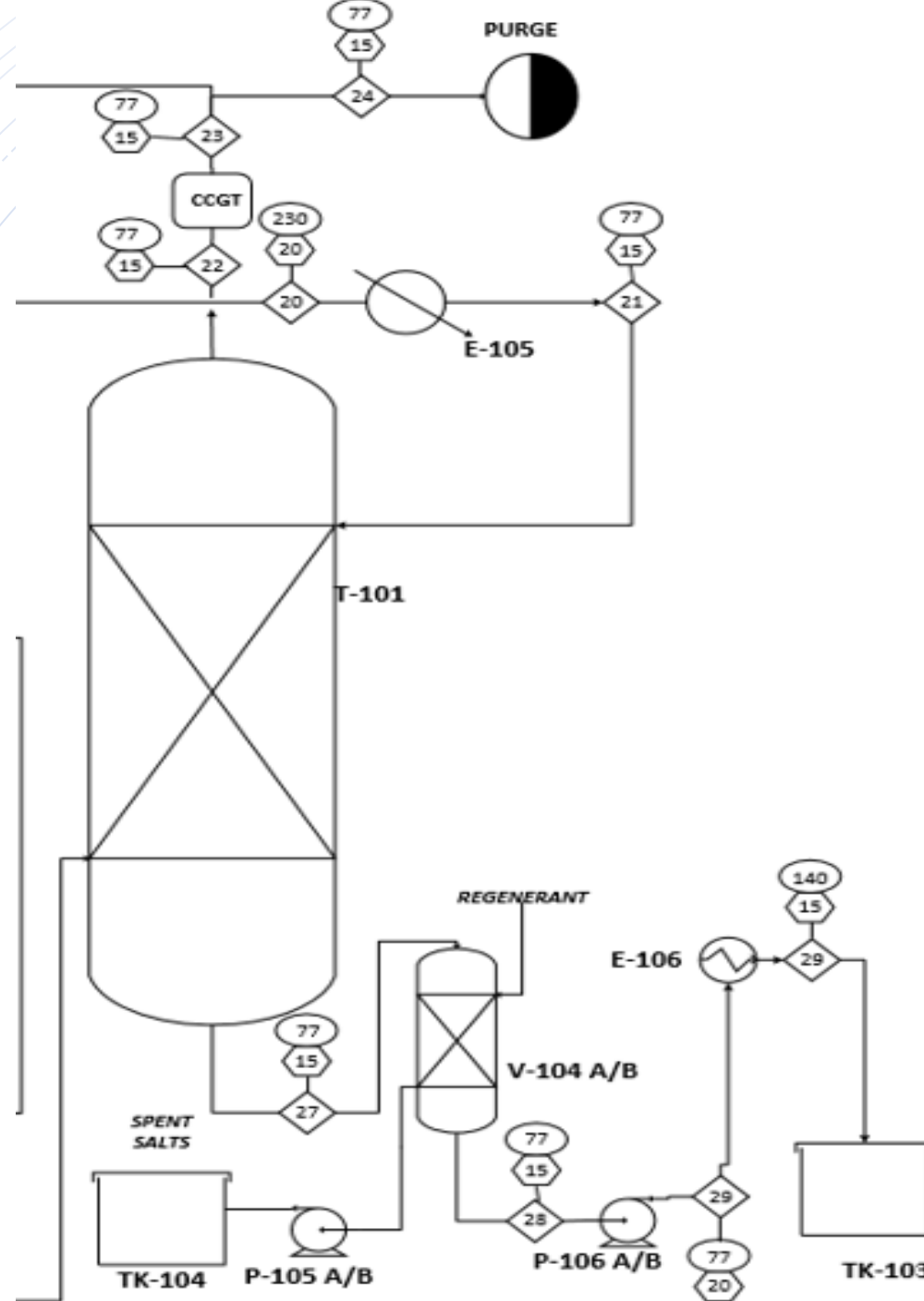
- Georgia Pacific
- Koch Industries Inc.

PFD

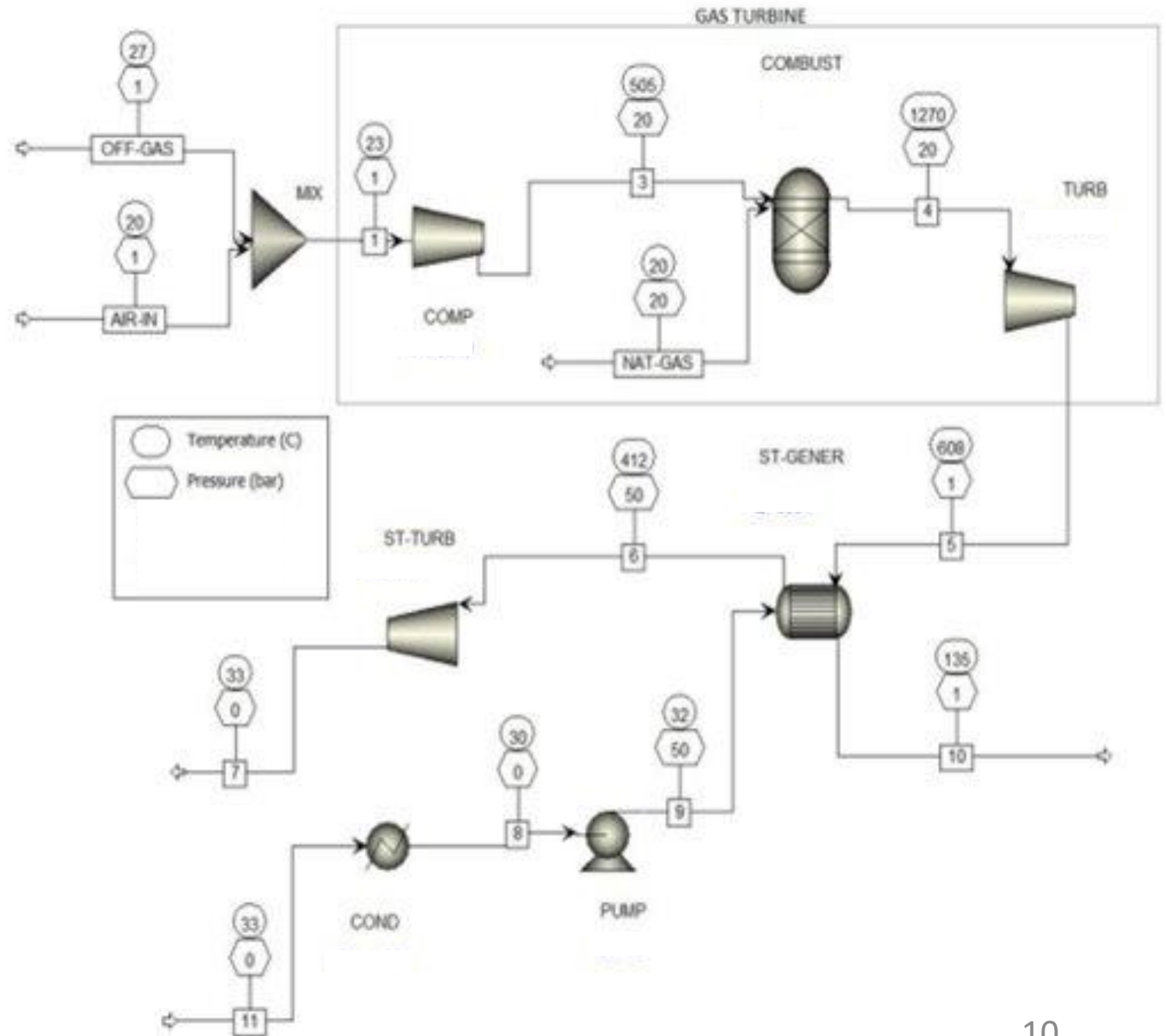
PFD
1/2



PFD 2/2

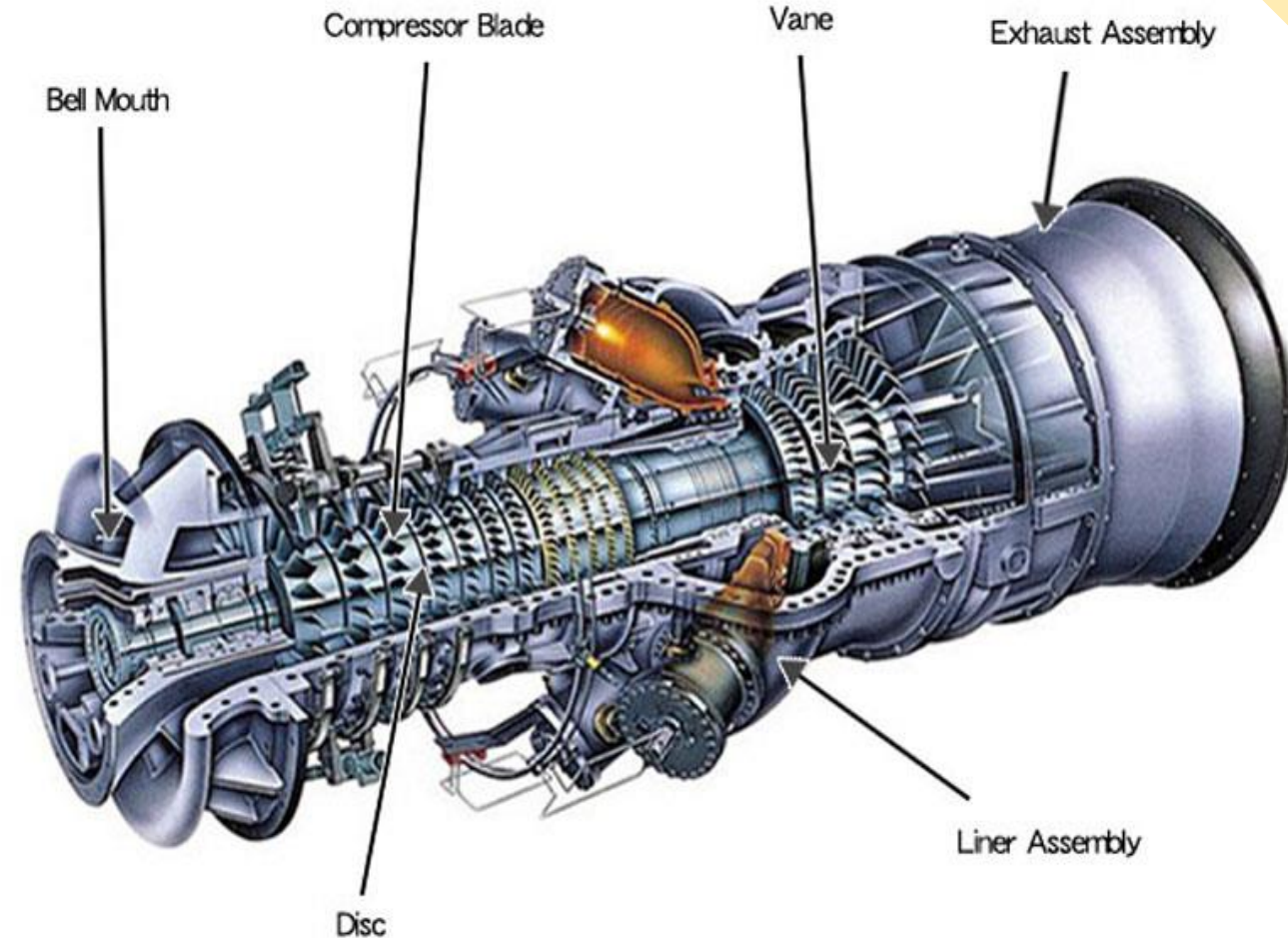


Combined-Cycle Gas Turbine (CCGT)

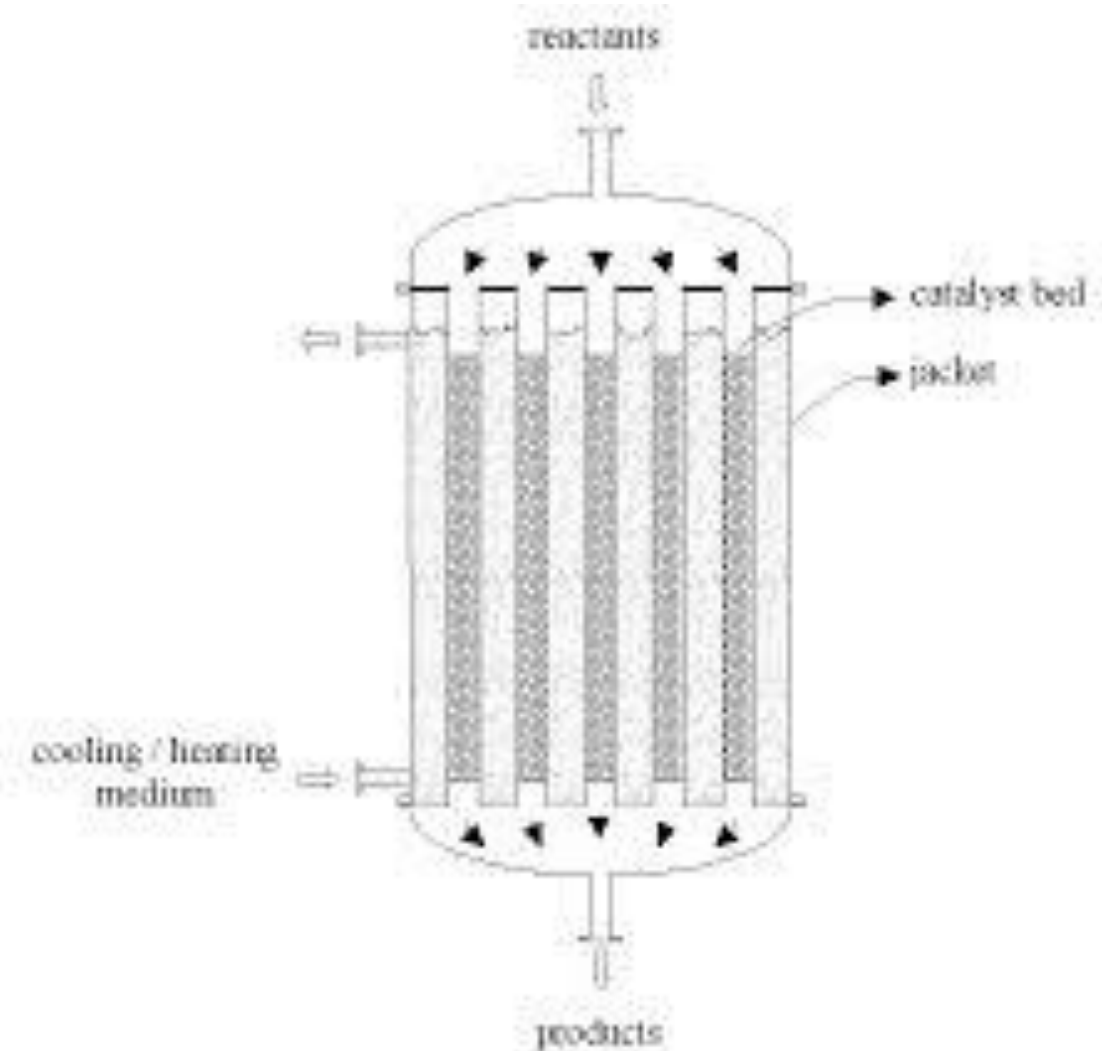


Combined-Cycle Gas Turbine (CCGT)

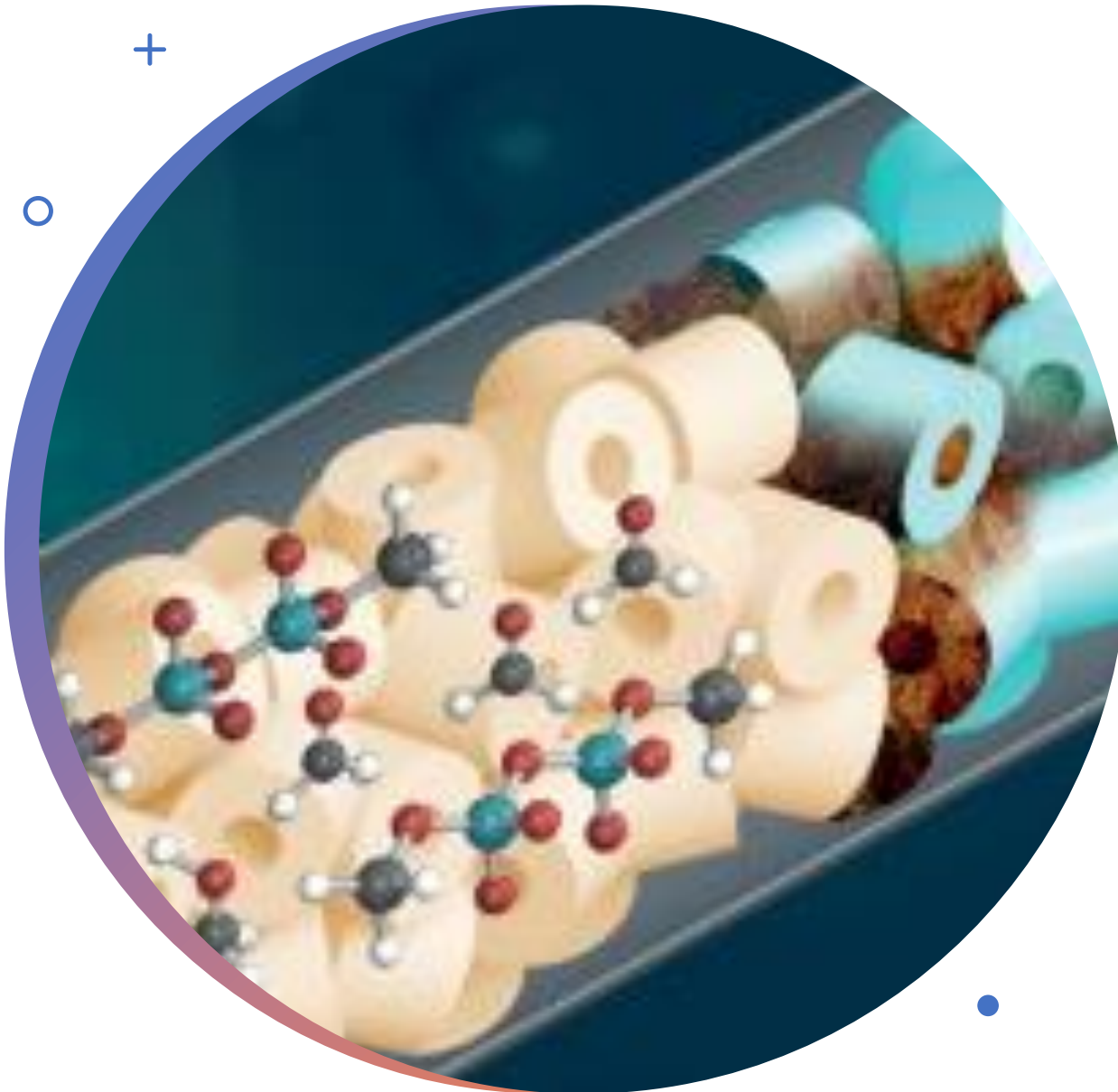
- Co-incineration with natural gas of waste gases with CCGT is used to remove formaldehyde and volatile organic compounds (VOCs) to 0.
- The CCGT recovers waste heat from turbine exhaust gas to generate steam providing electricity.
- Saves electricity cost needed to operate the formaldehyde production process.



Reactor Specification Sheet

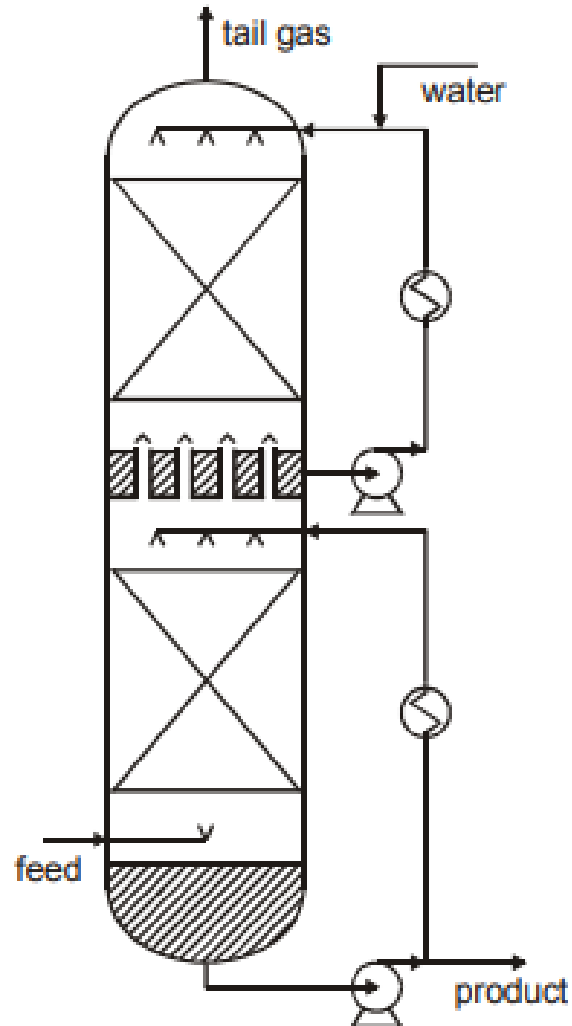


Reactor				
Identification:	Item:	Multi-Tubular Reactor		
	Item No:	R-101	Date:	4/21/2020
	No. Required:	1	By:	XW
	C _{PE} (\$)	\$ 146,000	C _{BM} (\$):	\$585,000
Function: To react methanol and oxygen to yield formaldehyde (product) and water (co-product).				
Operation: Continuous				
	Inlet	Outlet		
Materials Handled:				
Total Flow (lb/hr):	117,00	117,000		
Volumetric Flow (ft ³ /min)	1700	2500		
Component Flows (lbmol/hr):				
Formaldehyde	0	300		
Methanol	300	0		
Water	150	450		
Oxygen	300	150		
Nitrogen	3400	3400		
Temperature (°F):	518	545		
Pressure (psia):	22	15		
Vapor Fraction:	1.0	1.0		
Design Data:				
Q (MBTU/hr):	-800	Material:	Stainless Steel	
U _o (BTU/hr-ft ² -°F):	100	Design Temperature (°F):	660	
Total A _o (ft ²):	47	Design Pressure (psia):	50	
Tubes per Reactor	38	LMTD (°F):	174	
Tube Length (ft)	5			
Utilities:				
Dowtherm (lb/hr):	22,000			
Catalyst Data:				
Type:	Iron-Molybdenum	Density (lb/ft ³):	45	
Total Weight (lb):	11,000	Void Fraction:	0.60	
Catalyst Load (lb):	289			



- Material – Methanol and Formaldehyde does not react with Stainless Steel.
- Safe Temp. Operation Range is 480 F - 660 F. Operating at 518F allows hotspots at safe process temperatures; (above 660F formaldehyde oxidizes to CO by product – reduced plant productivity)
- Optimal presence of Steam – reduces Mo's consumption rate; too much water blocks active sites and diminishes methanol reduction
- Excess Oxygen in Feed – prevents removal of oxygen from catalyst surface during reaction
- Catalyst Function
 - $\text{Fe}_2(\text{MoO}_4)_3$ active phase
 - Excess MoO_3 ensures oxygen availability, improves formaldehyde selectivity, electron donor phase
 - Optimal yield and formaldehyde selectivity molar ratio ($\text{Mo/Fe} = 2.4$)

Absorption Column Specification Sheet



Absorber Column

Identification:	Item:	<i>Absorption Column</i>		
	Item No:	<i>T-101</i>	Date:	<i>4/21/2022</i>
	No. Required:	<i>1</i>	By:	<i>XW</i>
	CPE (\$)	<i>\$ 98,000</i>	CBM (\$):	<i>\$ 426,000</i>

Function: To separate most of the formaldehyde from the reactor effluent stream and provide the product stream to the product cooler.

Operation: Continuous

	Feed	Water	Purge	Product
Materials Handled:				
Total Flow (lb/hr):	117,000	81,000	101,000	17,000
Volumetric Flow (ft ³ /min)	1,450	130	308,000	294
Component Flows (lbmol/hr):				
Formaldehyde	300	0	16	284
Methanol	0	0	0	0
Water	450	450	0	450
Oxygen	150	0	150	0
Nitrogen	3,400	0	3,400	0
Temperature (°F):	230	77	77	77
Pressure (psia):	22	22	15	15
Vapor Fraction:	1.0	0.0	1.0	0.0

Column Design Data:				
Height of Column (ft):	33	Orientation:	Vertical	
Diameter of Column (ft):	7	Packing type:	Random	
Internals:	Ceramic Pall Rings	Void fraction:	0.92	
Height of Packing (ft):	25			
Column Material	Stainless Steel			
Design Pressure (psia):	50			
Design Temperature (°F):	300			

- Packed Column – continuous interaction of vapor and liquid phases, smaller pressure drop
- Ceramic Pall Ring packing (random) – reduces corrosion, chemically inert
- Improved Absorption/production of methylene glycol at higher pH (pH 8-9) – caustic wash addition to solvent
- External liquid recirculation with heat exchangers for tight temperature control





HAZOP

Nodes	Parameter	Guideword	Cause	Consequence	Action
Mixture Feed	Flow	No	Closed or failed feed valve	Build-up of pressure and chance of equipment failure/ destruction	Have the valve auto-fail to open to ensure flow and prevent a blockage of the flow
	Concentration	High	Excessive flow from feed	Potential for runaway reaction or explosion	N ₂ flush tank placed at reactor entrance to drop concentration
Reactor Tubes	Temperature	High	Heating element responsible for temperature control of reactor spikes	The reactor overheating can lead to a runaway reaction	Have a temperature control system to ensure temperature does not exceed limit.
	Pressure	Low	Blockage from catalyst degradation	Poor reaction efficiency	Follow maintenance schedule for catalyst bed
Dowtherm Inlet	Flow	Less	Partially closed valve	Enough heat of reaction might not be removed causing less products	Have a sensor that will monitor Dowtherm flowrate into the reactor

HAZOP Consequences and Actions

Main Parameters:

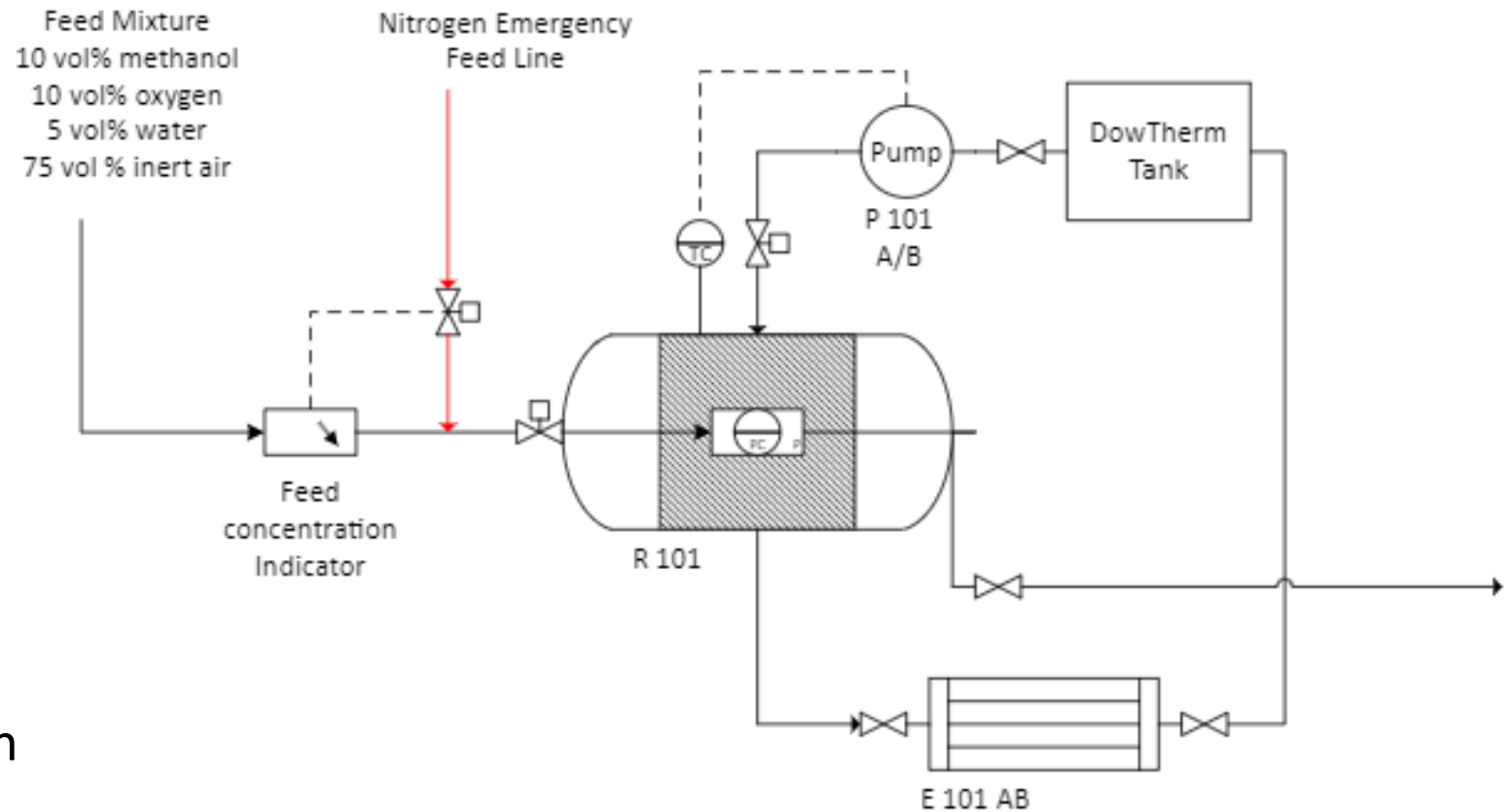
- Concentration
- Temperature

Consequences:

- Uncontrollable/runaway reaction
- Increased hotspot temperatures
- Build up of pressure

Actions:

- Nitrogen flush at reactor entrance
- Increase flow of dowtherm in shell



Major Safety Issues and Preventative Measures

- Deflagration Risk – flash fire within process

- Methanol flow meters
- Oxygen meters during normal operation
- Methanol accumulation – drain below the vaporizer
- Temperature measurements to detect fires
- No exposed catalyst on tube sheet after reloading
- Final safety: the rupture discs



- Paraformaldehyde Build-Up - Self-propagating, increases risk of deflagrations/fires, possible seizure of rotational equipment (absorber and process stream heat exchangers susceptible to build up)

- Tight temp control in absorption column (favor higher temps), ensure continual fluid flow (no stand stills)

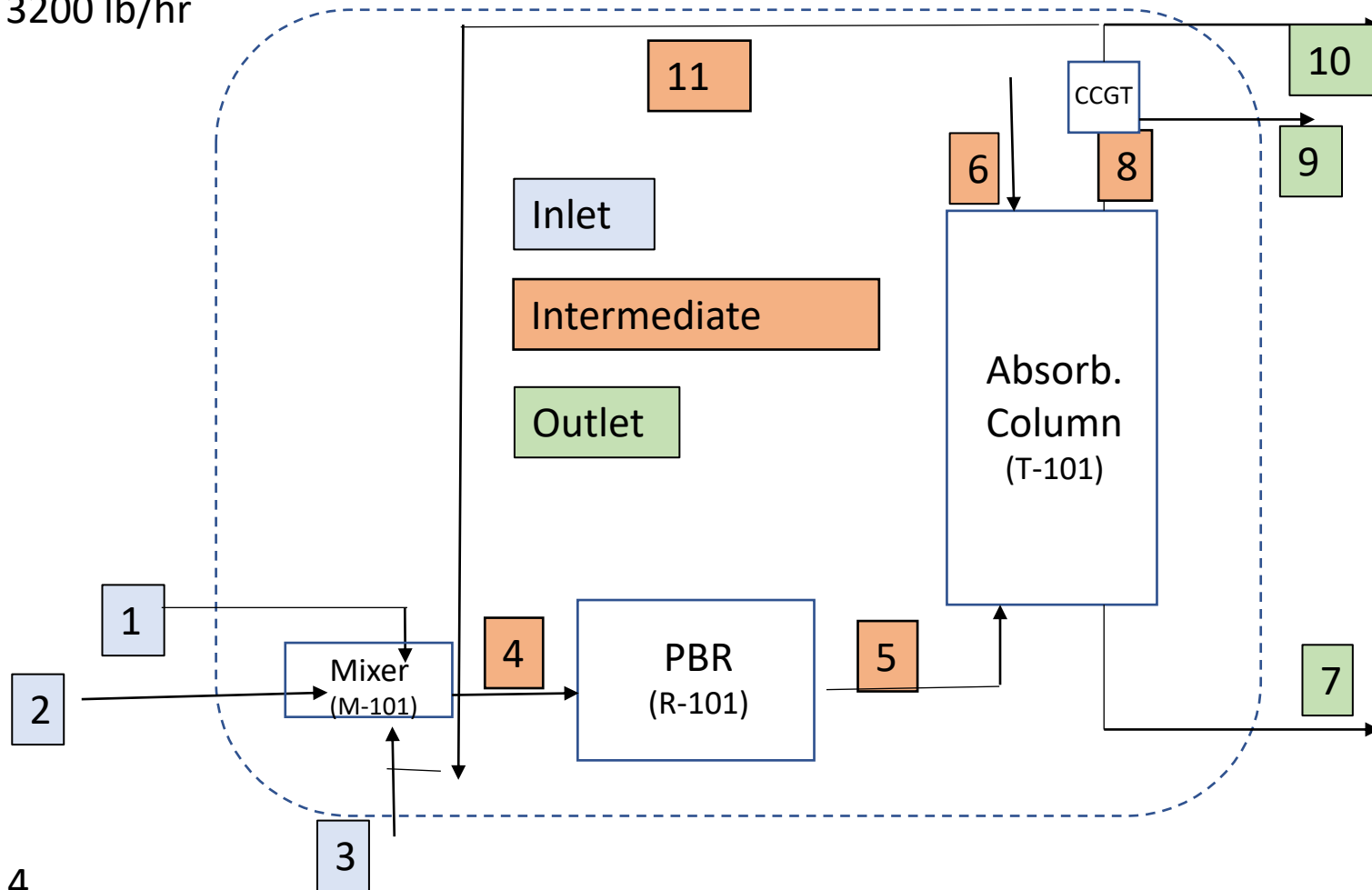
- HTF (DowTherm) Fires

- Check for tube leaks – pressurize HTF system, odor check then visually check for leaks if a smell is detected

Material and Energy Balance

Stream 11

- Inert recycle – 63000 lb/hr
- O₂ – 3200 lb/hr



Stream 4

- CH₃OH – 9600 lb/hr
- O₂ – 9600 lb/hr
- Inert air – 32000 lb/hr
- Inert recycle – 63000 lb/hr
- H₂O – 2700 lb/hr

Stream 5

- CH₂O – 9000 lb/hr
- H₂O – 8100 lb/hr
- Inert air – 95000 lb/hr
- O₂ – 4800 lb/hr

Stream 6

- $\text{H}_2\text{O} - 8100 \text{ lb/hr}$

Stream 8

- Inert air – 95000 lb/hr
- CH₂O – 470 lb/hr
- O₂ – 4800 lb/hr

Overall Balance

Stream 1 (In)

- $\text{H}_2\text{O} - 2700 \text{ lb/hr}$

Stream 2 (In)

- $\text{CH}_3\text{OH} - 9600 \text{ lb/hr}$

Stream 3 (In)

- O₂ – 6300 lb/hr
- Inert air – 31000 lb/hr

Stream 7 (Out)

- CH_2O – 8500 lb/hr
- H_2O – 8100 lb/hr

Stream 9 (Out)

- $\text{CH}_2\text{O} - 470 \text{ lb/hr}$

Stream 10 (Out)

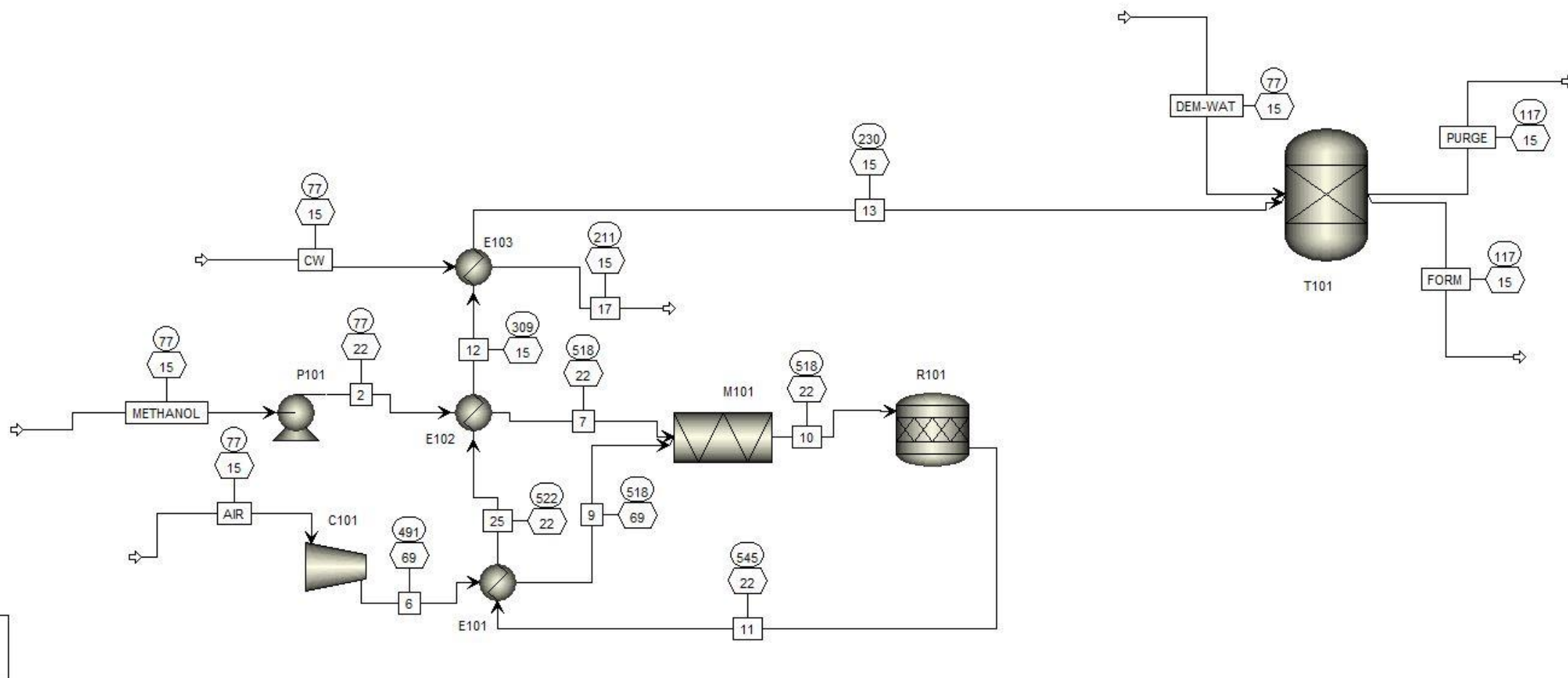
- Inert air – 32000 lb/hr
- O₂ – 1600 lb/hr

Total mass = 50000 lb/hr

Energy Balance

Equipment Name	MBtu/hr
Methanol Vaporizer (E-101)	4,500
Water Vaporizer (E-102)	7,600
Air Exchanger (E-103)	400
Absorption Column (T-101)	5.5
Reactor (R-101)	-800
Dowtherm Condenser (TK-102)	800

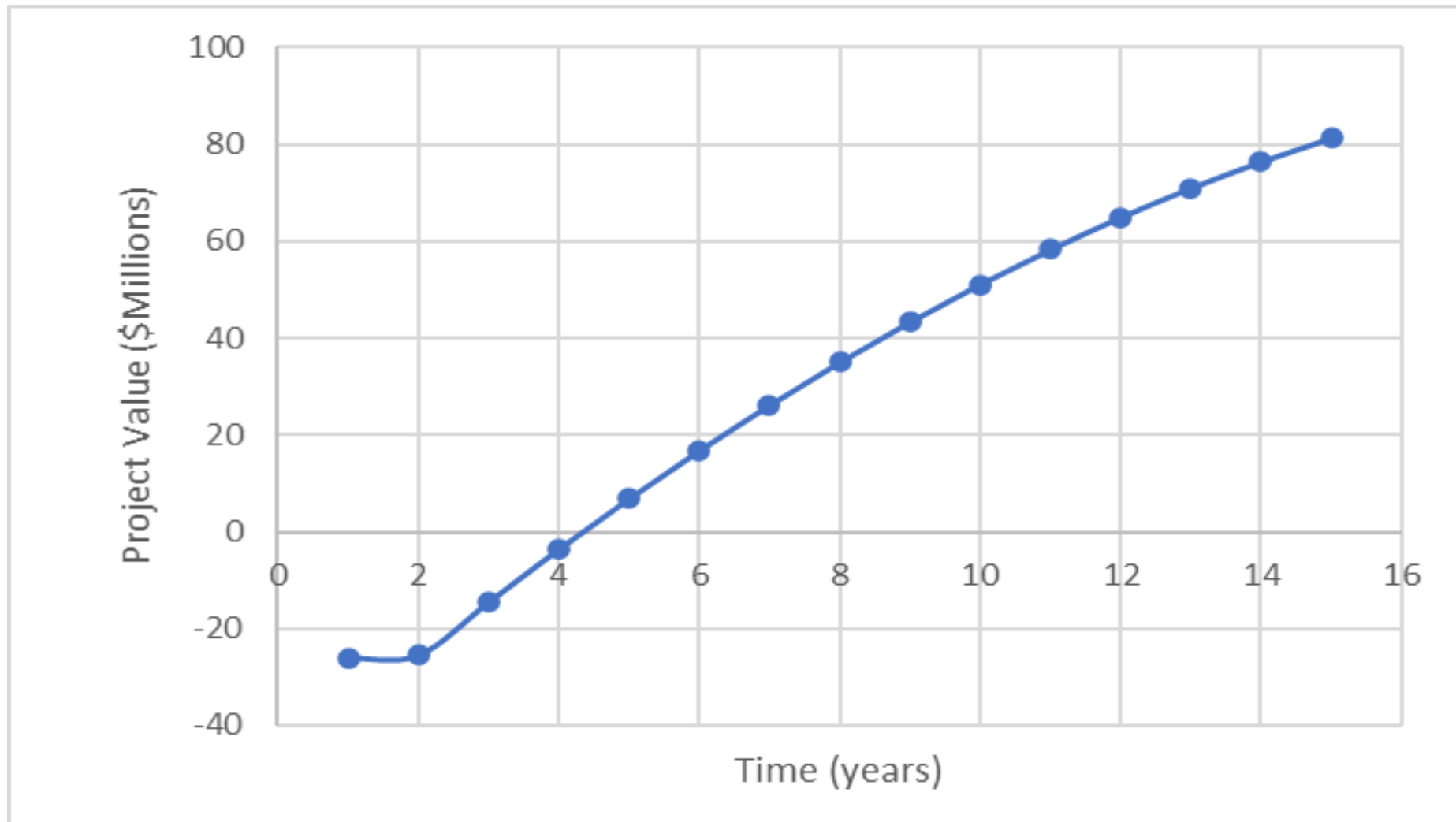
Aspen





Economics

Plant Cash Flow Diagram

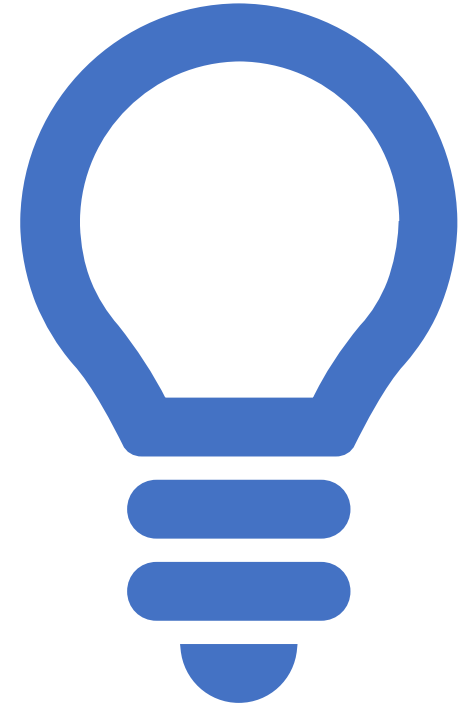


Production Cost (in millions)	
Raw Material Utility Operation	\$25.52/year
Production Revenue (in millions)	
Formalin	\$35.94/year
Difference Cost: \$10.42/year	
Total Investment (in millions)	
Fixed Capital Investment (FCI)	\$38.2
Working Capital	\$5.27
Total Investment	\$43.47

Profitability Analysis	
Plant Capacity (in millions)	120 lbs/year
Net Present Value (in millions)	\$210.77
Rate of Return on Investment (ROI)	28.8%
Payback Period	4.5 years
Discounted Cash Flow Rate of Return (DCRR)	10.00%

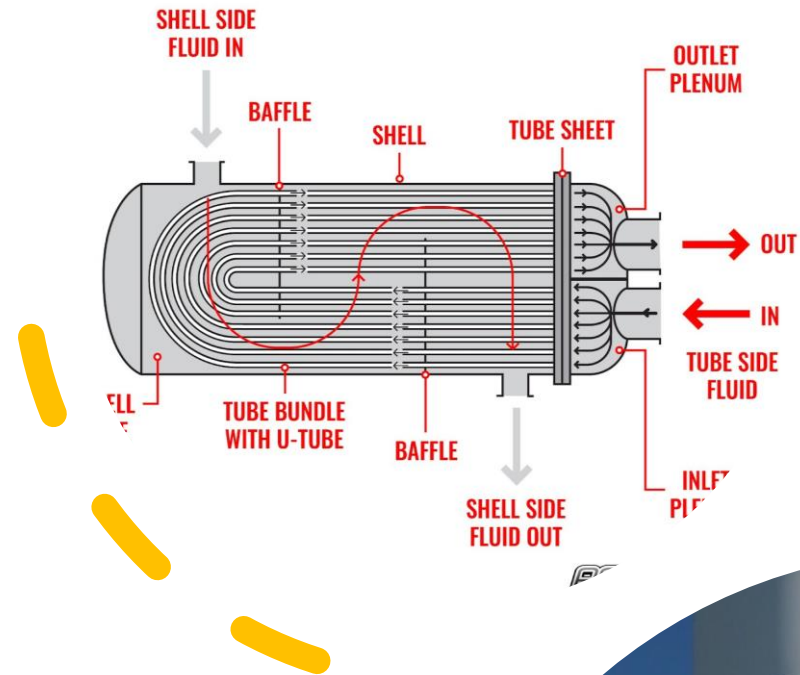
Future Recommendations

- Consider not moving forward with plant construction (unattractive payback period)
- Improve pressurization efficiency via Turbocharger
- Sell electricity back to the grid from total plant steam generation (dowtherm and CCGT) - increase profit



Start Up

- Twice a year
- Electric powered vaporizers and exchangers
- N₂ flush at entrance to reactor

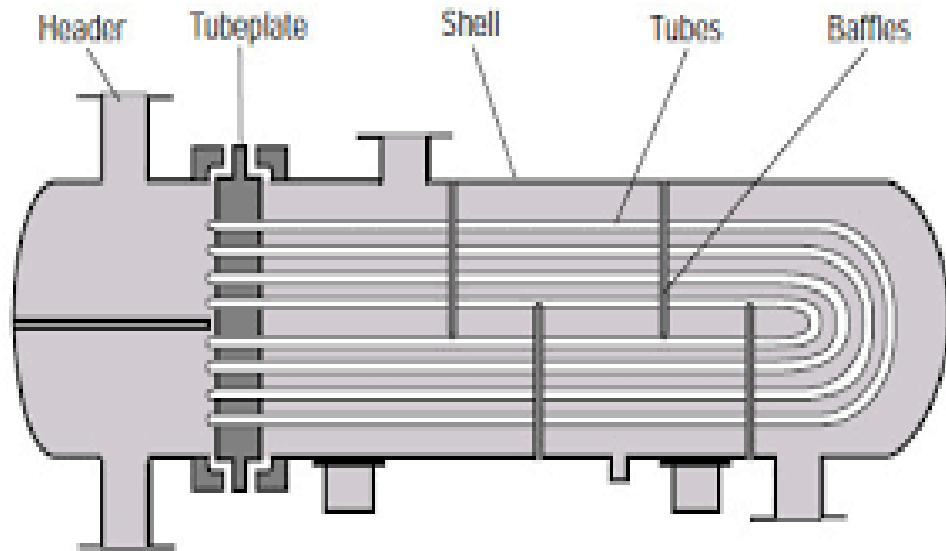


Longevity of Equipment/Maintenance

- Resistance to coking within reactor by adding water to the feed stream
- Operating under maximum capacity limit of equipment
- Remove Paraformaldehyde buildup during plant shutdown with caustic wash solution (1-2 wt%)
 - Manholes on absorber prevent pressurization and allow ventilation during cleaning
- Prioritize Proactive Work – Condition Based Maintenance
 - Vibration monitoring and analysis, control valve monitoring, Corrosion control, thermography
- Ensuring Methanol Quality
 - Poor quality methanol causes foaming in absorber



Methanol Vaporizer Specification Sheet



Methanol Vaporizer

Identification:	Item:	<i>Shell and Tube Heat Exchanger</i>		
	Item No:	<i>E-101</i>	Date:	<i>4/16/2020</i>
	No. Required:	<i>1</i>	By:	<i>HM</i>
	CPE (\$)	<i>\$ 233,000</i>	CBM (\$):	<i>\$ 1,440,000</i>

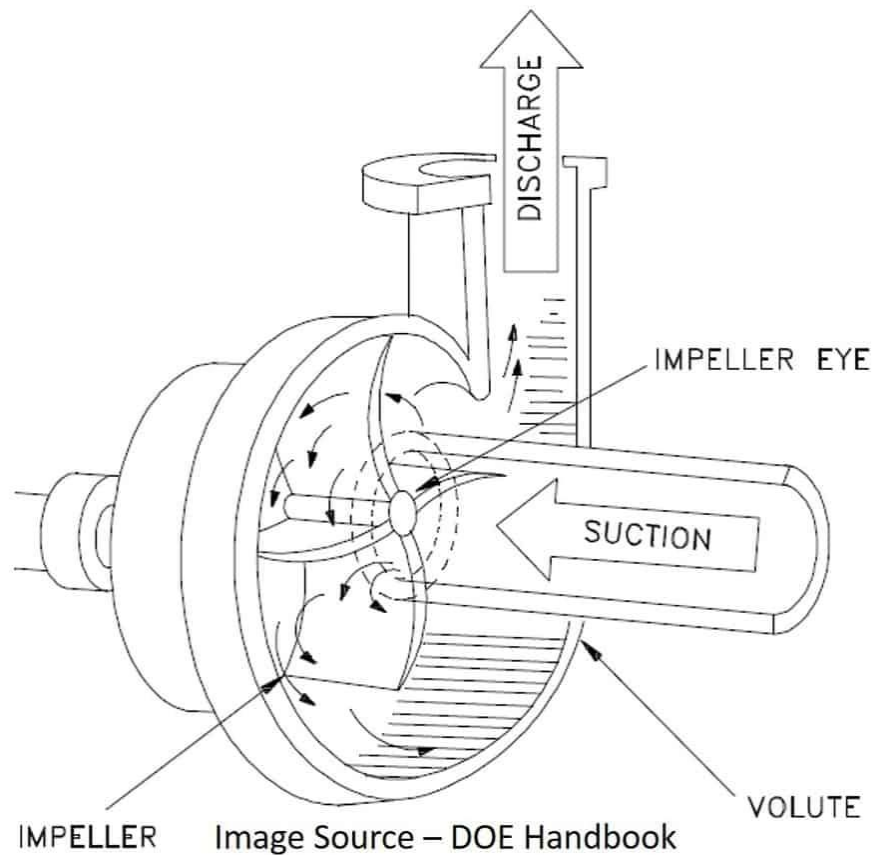
Function: To heat and vaporize methanol feed prior to entry into the static mixer and reactor.

Operation: Continuous

	Inlet	Outlet
Materials Handled:		
Total Flow (lb/hr):	9,600	9,600
Volumetric Flow (ft ³ /min)	196	196
Component Flows (lbmol/hr):		
Formaldehyde	0	0
Methanol	300	300
Water	0	0
Oxygen	0	0
Nitrogen	0	0
Carbon Monoxide	0	0
Temperature (°F):		
	68	518
Pressure (psia):		
	22	15
Vapor Fraction:		
	0.0	1.0

Design Data:				
Q (MBTU/hr):	4,500	Material:	Stainless Steel	
U _o (BTU/hr-ft ² -°F):	21	LMTD (°F):	125.0	
A _o (ft ²):	51,000			
Design Temperature (°F):	550			
Design Pressure (psia):	50			

Methanol Feed Pump Specification Sheet



Methanol Feed Pump

Identification:	Item:	<i>Centrifugal Pump</i>		
	Item No:	<i>P-101 A/B</i>	Date:	<i>4/18/2022</i>
	No. Required:	<i>2</i>	By:	<i>XW</i>
	CPE (\$)	<i>\$ 11,000</i>	CBM (\$):	<i>\$ 55,000</i>

Function: To pump methanol feed from 15 psia to 22 psia.

Operation: Continuous

	Inlet	Outlet
Materials Handled:		
Total Flow (lb/hr):	9,600	9,600
Volumetric Flow (ft ³ /min)	196	196
Component Flows (lbmol/hr):		
Formaldehyde	0	0
Methanol	300	300
Water	0	0
Oxygen	0	0
Nitrogen	0	0
Carbon Monoxide	0	0
Temperature (°F):	68	68
Pressure (psia):	15	22
Solid Fraction by Volume:	0.0	0.0

Design Data:				
Flow Rate (gpm):	660			
ΔP (psia):	7			
Material:	Stainless Steel			
Hydraulic Power (hp):	4			
Shaft Power (hp):	5			

Utilities:				
Electricity (kW):	4			

Process Selection

Attribute	Weight	Silver Catalyst Process	Score	Metal Oxide Catalyst Process	Score
Conversion	0.20	85% conversion	85	99% conversion	100
Catalyst Life	0.05	3 -4 months, regeneration, expensive, relatively instable	40	Lifespan 12 - 18 months, regeneration not practical, economical, relatively stable	60
Risk	0.20	Operates ABOVE explosion limit, requires very high reactor temperatures	50	Operates BELOW explosion limit, oxygen in absorber increases fire risk, hot oil used, increases fire risk	40
Steam Production	0.05	Insufficient steam production to meet plant power needs	40	Sufficient Steam Production to meet plant power needs	80
Environmental Impact	0.05	1.55 kg/MG uncontrolled CH2O emissions; 0.2% formladehyde in steam condensate	30	0.98 kg/MG uncontrolled Formaldehyde emissions	70
Product Quality	0.15	More Impurities	30	Less Impurities, higher obtainable concentration, specialized products	90
Utility Cost	0.10	\$1.65 M/Year	70	\$2.3 M/Year	50
Capital Cost	0.10	\$7.1 M	50	\$6.2 M	70
Installation Cost	0.05	High installation cost	20	Low installation cost	100
Payback Period	0.05	2.8 years	70	3.5 years	50
Total	1.00		53.5	33	71.5

Plant Ion Exchange

Deionization of Water

Deionization of Formalin Stream

- Polystyrene-divinylbenzene resin
- Strong Base Anion
- Resin Regeneration

SENIOR DESIGN AND PROFESSIONALISM II SPRING 2022

HOMEWORK 1

SENIOR DESIGN AND PROFESSIONALISM II SPRING 2022

CHEG 4248 Senior Design & Professionalism II Spring 2022: Home Work 1

**February 10, 2022
Due: February 17, 2022**

You will be graded based on your ability to function as a member of a design team. Include minutes of meetings, assignment of tasks and confidential evaluation of group members on forms previously provided. Clarity of presentation is essential if you are to avoid losing points.

- (a) Create a list of major tasks and their respective duration to be accomplished to enable you achieve the goals and objectives for your project**
- (b) Organize the tasks into phases/module**
- (c) Identify sub-tasks and their respective duration**
- (d) Link major tasks and/or sub-tasks when required**
- (e) Identify milestones and deadlines to track an important event**
- (f) Prepare a Gantt Chart print out using Microsoft Project or Excel**

**DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM II CHEG 4248
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR SPRING 2022 SEMESTER**

ABET Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.

Assignments that test competency in this area will include problems that test a student's ability to (1) accommodate the needs of others, (2) share responsibilities, (3) commit to team goals, (4) apply principles of constructive conflict management to interaction with others, (5) support members, and (6) communicate with team members.

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Max for this Assignment	Your Score
Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.		
Ability to follow good team management practices and resolving conflicts <i>Plan group meetings and time management, distribute project tasks evenly,.</i>	50	
An ability to track and meet project schedule <i>Evaluate performance of team members on a regular basis, and track progress of team members</i>	50	
TOTAL	100	

ABOVE AVERAGE

Above Average Student Original Graded Assignment on Home Work #1

CHEG 4248 Senior Design & Professionalism II Spring 2022: Homework 1

February 10, 2022

Due: February 17, 2022

You will be graded based on your ability to function as a member of a design team. Include minutes of meetings, assignment of tasks and confidential evaluation of group members on forms previously provided. Clarity of presentation is essential if you are to avoid losing points.

- (a) Create a list of major tasks and their respective duration to be accomplished to enable you to achieve the goals and objectives for your project**
- (b) Organize the tasks into phases/module**
- (c) Identify sub-tasks and their respective duration**
- (d) Link major tasks and/or sub-tasks when required**
- (e) Identify milestones and deadlines to track an important event**
- (f) Prepare a Gantt Chart print out using Microsoft Project or Excel**

93%

**DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM II CHEG 4248
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR SPRING 2022 SEMESTER**

ABET Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.

Assignments that test competency in this area will include problems that test a student's ability to (1) accommodate the needs of others, (2) share responsibilities, (3) commit to team goals, (4) apply principles of constructive conflict management to interaction with others, (5) support members, and (6) communicate with team members.

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Max for this Assignment	Your Score
Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.		
Ability to follow good team management practices and resolving conflicts <i>Plan group meetings and time management, distribute project tasks evenly,.</i>	50	47
An ability to track and meet project schedule <i>Evaluate performance of team members on a regular basis, and track progress of team members</i>	50	46
TOTAL	100	93

Simplified Guide for End of Spring Semester Report

Assignment Title: Homework 1

Due Date: February 17, 2022

Team Members: Willie Conner, Chinenye Ihe, Utomwen Irabor, Shimere Gregory

MAJOR TASKS

- | | |
|---|-----------|
| 1. Plant and Production Capacity Increase | (1 day) |
| 1. Visio and ASPEN completion | (2 weeks) |
| 2. Economic Evaluation | (4 weeks) |
| 3. HAZOP and safety | (2 weeks) |
| 4. Final Written Report | (2 weeks) |

PHASES/MODULES

1. Phase 1 – Plant and Production Capacity Increase
2. Phase 2 – Visio and ASPEN completion
3. Phase 3 – Economic Evaluation
4. Phase 4 – HAZOP and Safety
5. Phase 5 – Final Written Report

SUB-TASKS

- | | |
|--------------------------------------|--|
| 1. Fall Semester Review | (January 18 th – 25 th) |
| • Plant Production Increase | (January 18 th – 20 th) |
| • Plant Capacity Increase | (January 20 th – 22 nd) |
| • Recalculate Material Balance | (January 23 rd – 25 th) |
| 2. HYSYS/ASPEN Simulation of Process | (January 25 th – Feb. 10 th) |
| • Converge the Simulation | (February 1 st – 8 th) |
| • Recalculating Energy Balance | (February 8 th – 10 th) |
| 3. Chemical Engineering Design | (February 10 th – March 3 rd) |
| • Design of Major Equipment | (February 10 th – 20 th) |

- | | |
|---|--|
| • Listing Equipment and Specification | (February 21 st – March 3 rd) |
| 4. Economic Evaluation | (March 3 rd – 23 rd) |
| • Raw Material costs | (March 3 rd – 12 th) |
| • Other variable costs | (March 12 th – 15 th) |
| • Fixed costs | (March 16 th – 18 th) |
| • Transportation costs | (March 19 th – 20 th) |
| • Cash flow and profitability analysis | (March 20 th – 22 nd) |
| • Summary | (March 22 nd – 23 rd) |
| 5. Safety and HAZOP Analysis | (March 23 rd – April 4 th) |
| 6. Reporting | (April 5 th – April 23 rd) |
| • Homework Assignments | (January 18 th – April 23 rd) |
| • Weekly meetings/reports with Dr. Dada | (January 23 rd – April 20 th) |
| • Midterm Report | (February 26 th – March 2 nd) |
| • Final Presentation Prep | (April 20 th – 22 nd) |



MAJOR MILESTONES

- | Milestones | Deadlines |
|--------------------------------------|----------------------------------|
| • Converge Aspen HYSYS Simulations | February 8 th , 2022 |
| • Design Major Equipment | February 20 th , 2022 |
| • Complete Economic Evaluations | March 23 rd , 2022 |
| • Complete Safety and HAZOP Analysis | April 4 th , 2022 |
| • Midterm Report | February 26 th , 2022 |
| • Final Presentation | April 23 rd , 2022 |
| • Final Report | May 1 st , 2022 |

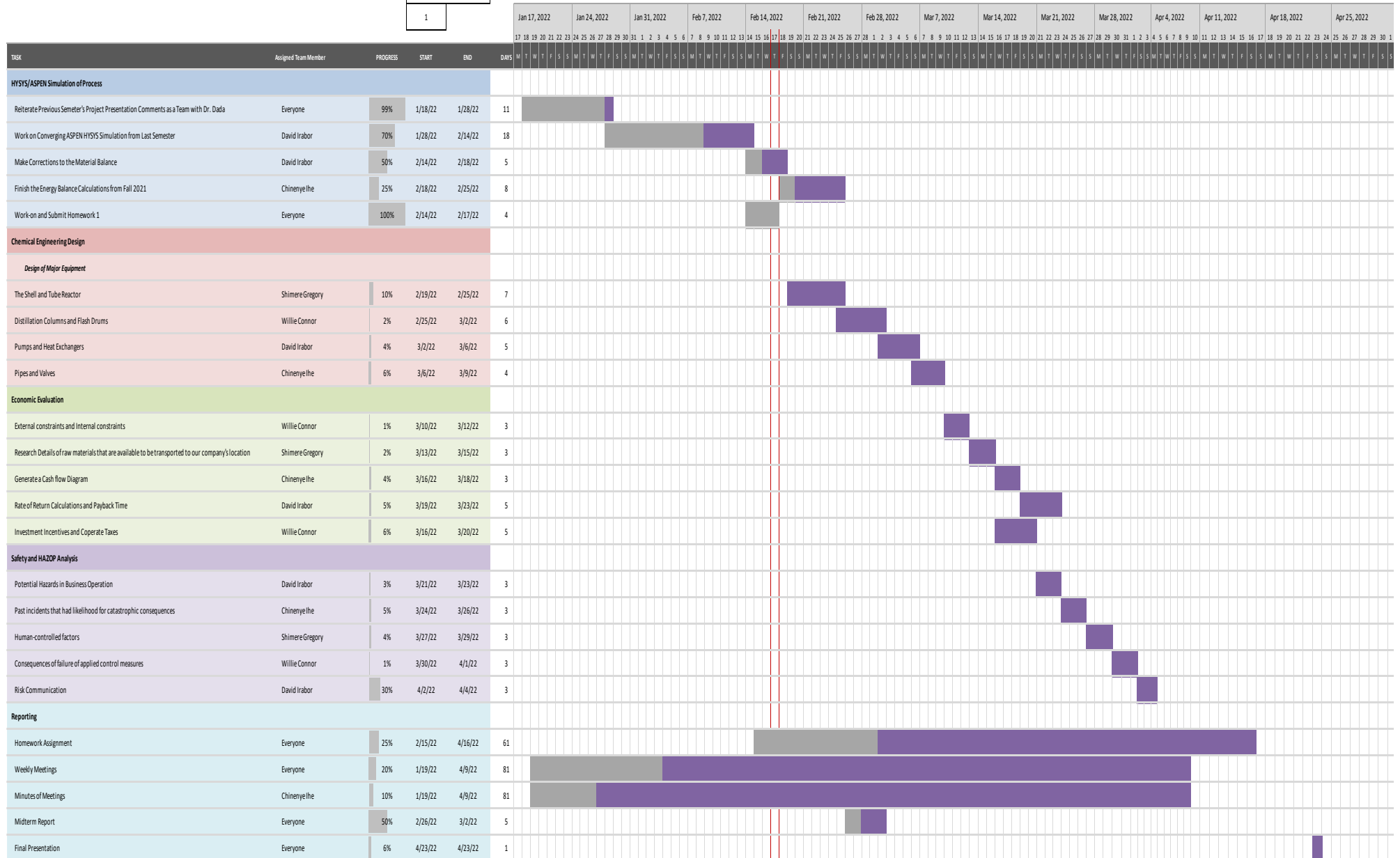
The Production of Propylene Oxide

Company: The Coperations

Project Team: Chinenye Ihe, Shimere Gregory, Utomwen Irabor, and Willie Conner

GANTT CHART

Due April 23rd, 2022	
Tuesday, January 18, 2022	
1	



OK ✓

CHEG 4248 Confidential TEAM Member Evaluation
PROJECT TITLE: Production of Propylene Oxide

TEAM #: **2** ASSIGNMENT/HOMEWK#: **1** LAST NAME: **Ihe** FIRST NAME: **Chinenye**

Directions: Fill out the evaluation for EACH member of your team in the correct column. **PLEASE INCLUDE YOURSELF.** Rate the performance of each student in each category on a 5-point scale (1 - Pathetic, 2 - Poor, 3 - Fair, 4 - Good, 5 - Excellent).

Names: A: Chinenye Ihe

B: Utomwen Irabor

C: Shimere Gregory

D: Willie Conner

E.

F:

Evaluation:

1. Student attended and contributed to the group meetings.

A: 5 B: 5 C: 5 D: 1 E: F:

2. Student performed his/her assigned tasks in a timely manner.

A: 5 B: 5 C: 5 D: 1 E: F:

3. Student performed technical tasks in a quality manner.

A: 5 B: 5 C: 5 D: 1 E: F:

OK

4. Student contributed to setting weekly goals and dates for tasks.

A: 5 B: 5 C: 5 D: 1 E: F:

5. Student was willing to work toward the benefit of the group.

A: 5 B: 4 C: 4 D: 4 E: F:

6. Student kept up to date with current project progress and logbook.

A: 5 B: 4 C: 4 D: 4 E: F:

7. Rate the overall performance of the student as a member of the team on this project.

A: 5 B: 5 C: 5 D: 2 E: F:

CHEG 4248 SENIOR DESIGN AND PROFESSIONALISM II
SPRING 2022
PROJECT ASSIGNMENT COVER SHEET

TEAM NUMBER: 2

ASSIGNMENT #: 1

Assignment Title: Homework 1

Due Date: February 17, 2022

No	TEAM Member Name TEAM Member Signature	Brief Description of Work Assigned to Member	% Completed by Member*	Your Score
1	Chinenye Ihe	Started Homework 1	100	100
2	Shimere Gregory	Completed Gantt Chart	100	100
3	Utomwen Irabor	Worked on Homework 1 and Process Flow Diagram	100	100
4	Willie Conner	Worked on minutes of meeting	100	100

*100% means the member completed his/her assigned work.

By signing this assignment cover sheet, I agree that the percentages stated in the % completed column reflect the contribution made by me and other members of the group.

CHEG 4248 SENIOR DESIGN AND PROFESSIONALISM I SPRING 2022

MINUTES OF TEAM MEETINGS

Meeting Date: 02/17/2022 Meeting Time: 10:40am Meeting Location: Zoom

Members Present: Chinenye Ihe, Utomwen Irabor, Shimere Gregory, Willie Conner

Agenda for Meeting (List all items to be discussed or discussed at the meeting)

- ✓ PFD corrections
- ✓ Homework 1/ Gantt Chart
- ✓ Assign Equipements

Detailed Minutes: (should include name of speaker and summary of what he/she suggested)

David was the speaker of the meeting, and he went over to the process flow diagram from last semester to make correctios for this semester and divided the tasks between all members of the team. He suggested that we should start to focus more on our equipment sizing for next week so that we can start on calculations.



CHEG 4248 SENIOR DESIGN AND PROFESSIONALISM II SPRING 2022

TASK ASSIGNMENT & DELIVERABLES AT MEETINGS

Use this table to document tasks assigned and deliverables completed/submitted by each group member at each meeting. If deliverables are not completed, indicate the actions taken by the group on this individual

Meeting Date: February 17, 2022 Meeting Time: 10:40am Meeting Location: Zoom

Name	Task Assigned	Deliverables Completed & Submitted
Chinenye Ihe	Start/Add to homework 1	Started homework 1, identified major tasks, phases, and sub-tasks
Shimere Gregory	Add Gantt Chart	Completed the Gantt Chart with all tasks and start to finish dates
Willie Conner	Helped to complete the minutes of meeting	Fixed grammatical errors on Homework 1 and wrote the minutes of meeting
Utomwen Irabor	Complete Homework 1	Completed homework 1

CHEG 4248 SENIOR DESIGN AND PROFESSIONALISM II

SPRING 2022

CLASS ATTENDANCE SHEET

This table documents attendance of students of the Senior Design & Professionalism class as indicated below and will be used to evaluate the sub outcome of ABET criterion 4 Students understanding and demonstration of professional responsibilities.

Meeting Date: February 17, 2022

Meeting Time: 10:40am

Meeting Location: Zoom

Student Name	Project Title	On time	5 minutes late	Absent
Utomwen Irabor	Homework 1	✓		
Chinenye Ihe	Homework 1	✓		
Shimere Gregory	Homework 1	✓		
Willie Conner	Homework 1			✓

AVERAGE

Average Student Original Graded Assignment on Home Work 1

Prairie View A&M University

Roy G. Perry College of Engineering Department:

Spring 2022



85%

Chemical Engineering CHEG 4247-P01

Senior Design & Professionalism

Homework #1

Date Due: February 17, 2022

Submitted by:

Group #1: Mohamed Akinotcho, Duaa Albadri,

Cayla Alexander, Jevaun Christie, Au'Myia Collins

Submitted to:

Dr.Dada

CHEG 4247 - Senior Design & Professionalism I (Fall 2021):

Homework 1

February 15, 2022

Due: February 17, 2022

You will be graded based on your ability to define and plan the project. Clarity of presentation is essential if you are to avoid losing points.

- (a) Create a list of major tasks and their respective duration to be accomplished to enable you achieve the goals and objectives for your project**
- (b) Organize the tasks into phases/module**
- (c) Identify sub-tasks and their respective duration**
- (d) Link major tasks and/or sub-tasks when required**
- (e) Identify milestones and deadlines to track an important event**
- (f) Prepare a Gantt Chart and print it out using Microsoft Project or Excel**

**DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM II CHEG 4248
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR SPRING 2022 SEMESTER**

ABET Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.

Assignments that test competency in this area will include problems that test a student's ability to (1) accommodate the needs of others, (2) share responsibilities, (3) commit to team goals, (4) apply principles of constructive conflict management to interaction with others, (5) support members, and (6) communicate with team members.

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Max for this Assignment	Your Score
Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.		
Ability to follow good team management practices and resolving conflicts <i>Plan group meetings and time management, distribute project tasks evenly,.</i>	50	43
An ability to track and meet project schedule <i>Evaluate performance of team members on a regular basis, and track progress of team members</i>	50	42
TOTAL	100	85

Overview

Project: Production of 1,3 butadiene from ethanol

- **How much is the major equipment for the process? Design/ Sizing?**
- **What is the type/cost of utilities?**
- **Determining estimate of fixed capital cost**
- **Manufacturing and production cost**
- **Develop economic analysis**
- **Create PFD, MEB, Specification sheet- all while using ASPEN software**

(a) Create a list of major tasks and their respective duration to be accomplished to enable you achieve the goals and objectives for your project

Major Tasks-

- ASPEN HYSYS (approx. 2- 3 weeks)
- Design of Major Equipment (approx. 3-4 weeks)
- Economic Analysis (approx. 3 weeks)
- Reporting (approx. 2 months)

(b) Organize the tasks into phases/module

Modules/Phases

Module 1: ASPEN HYSYS

Module 2: Major Equipment Specifications

Module 3: Economic Analysis

Module 4: Reporting

(c) Identify sub-tasks and their respective duration & (d) Link major tasks and/or sub-tasks when required

Sub-tasks

A. ASPEN HYSYS

Identify Process (approx. 2 days)

i. Fluid selection package, physical properties

ii. Determine types of streams, placement of flow lines, equipment, process data, etc.

- Energy Streams
- Material Streams
- Materials Specification

iii. Define Assumptions

Converge Process (approx. 1 week):

i. Understanding the connection between major units in the overall system.

Results of Simulation (approx. 1.5 weeks):

i. Specification Sheet: type/cost of equipment, types of material, sizing, location of equipment, unit variables, etc.

ii. Characteristics: Reliability of process and process variables

iii. Conditions: Pressure, temperature, concentration, volume, reactants, catalysts/process outcomes, and components

B. Major Equipment Specifications

Design of each major equipment (approx 2-3 week):

i. Identify what important/major units needed within the plant and how many there are desired

Detailed information (approx. 1 week):

i. inputs, outputs, recycle streams, equipment layout (instrumentation, streams, vessels, reactors, heat exchanger, distillation column) layout, process description, etc.

C. Economic Analysis

I. Capcost: (approx. 1 week)

i. Given the specification you want for your units, helps to determine cost of equipment that you are design

II. Cost Evaluation: (approx. 1 week)

i. Determines our direct cost such as service facilities, piping, electrical systems, indirect cost, and your fixed capital investment.

III. Develop Cash Flow (approx. 1 week)

i. ROI, IRR, NPV, DCFROR, and DPBP

D. Reporting

- Homework assignments (Every week)
- Midterm progress report (TBD)
- End of the semester report (April 16, 2022)
- End of the semester presentation (April 16, 2022)

(e) Identify milestones and deadlines to track an important event

Milestones

1. ASPEN HYSYS:(March 6, 2022)
2. Major Equipment Specifications: (March 2, 2022)
3. Economic Analysis: (March 31,2022)
4. Midterm Report: (March 7,2022)
5. Final Presentation: (April 11, 2022)

Deadlines

1. Assignments: (TBD)
2. Midterm Report: (March 9,2022)
3. Final Presentation (April 16, 2022)

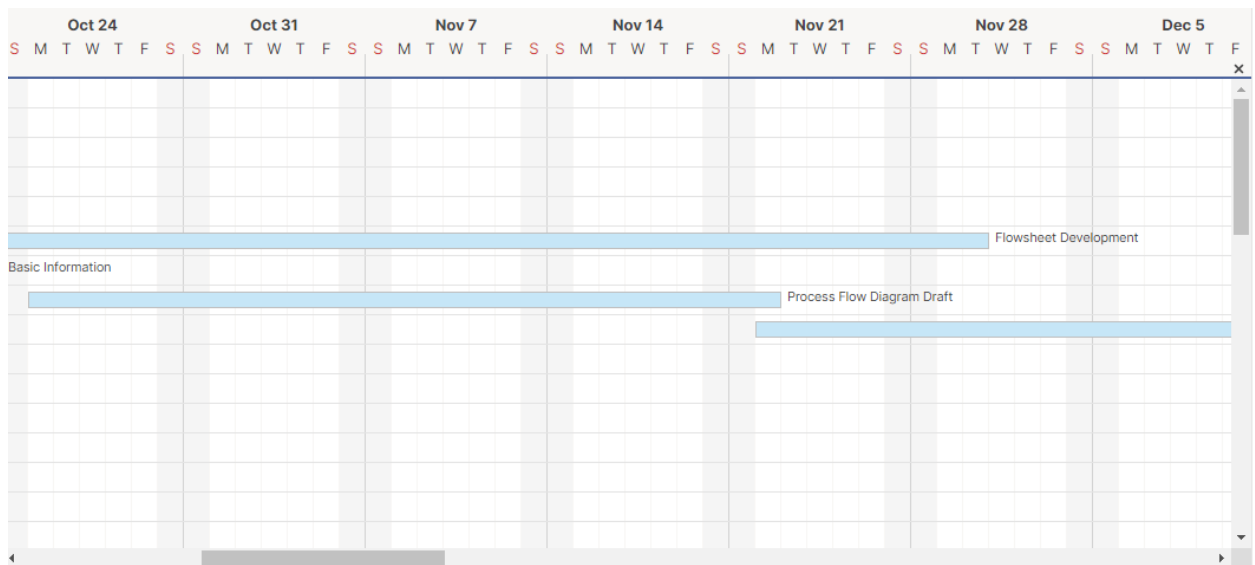
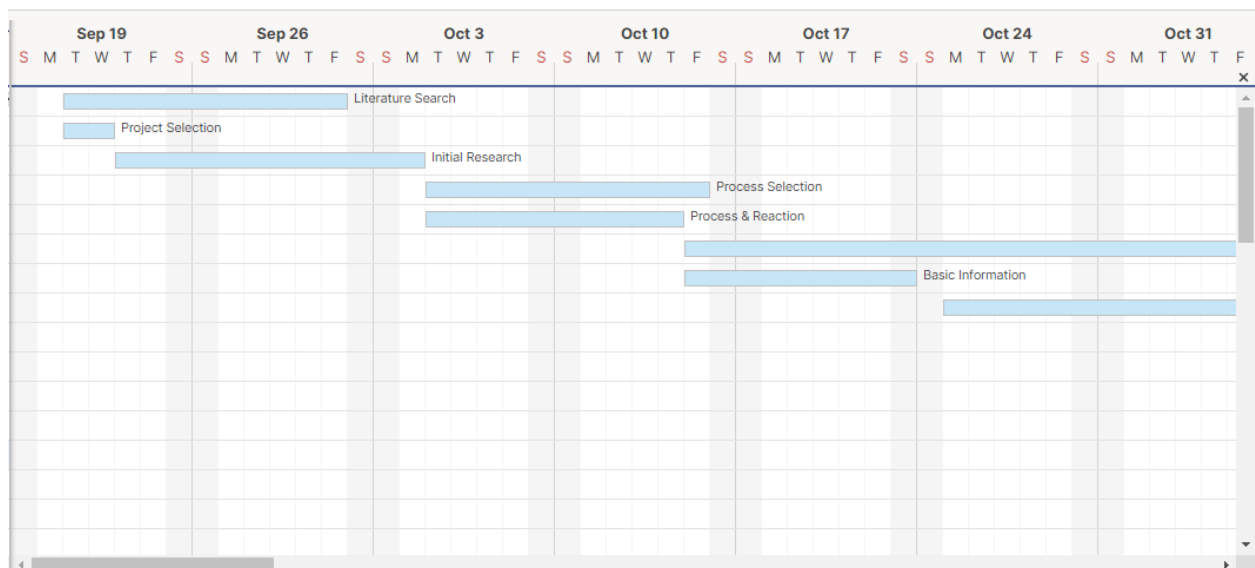
(f) Prepare a Gantt Chart print out using Microsoft Project or Excel

Please reference the Gantt Chart attached below:

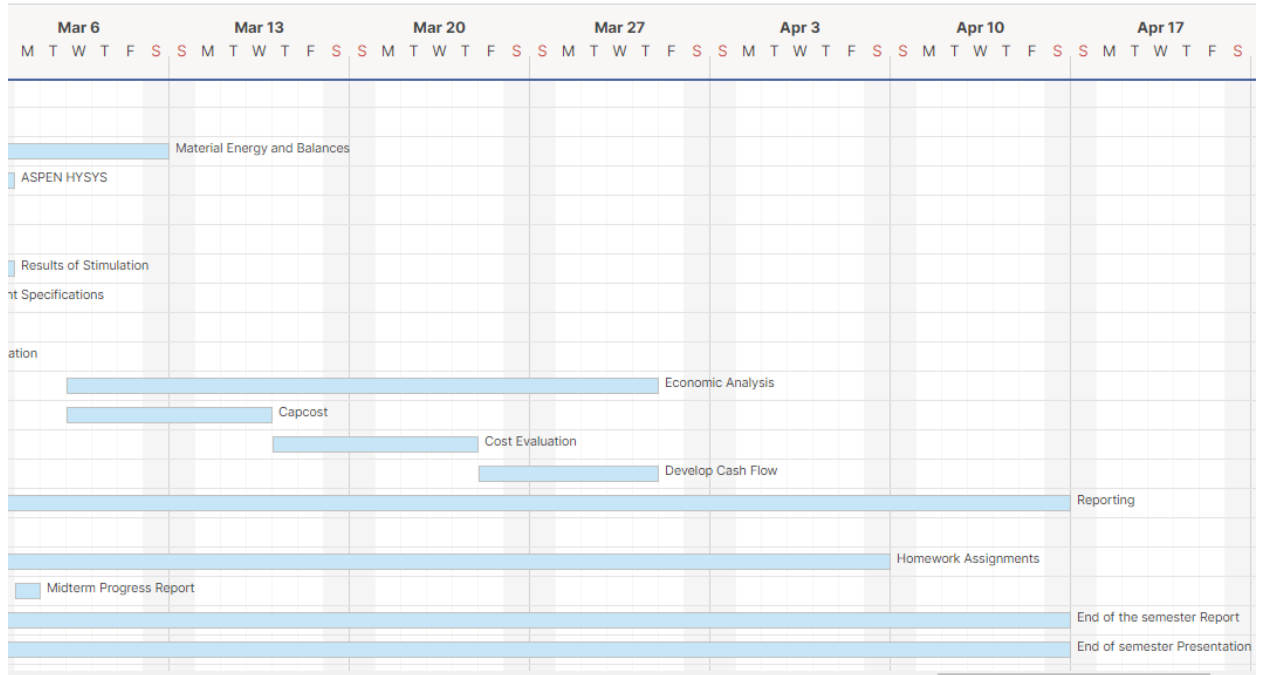
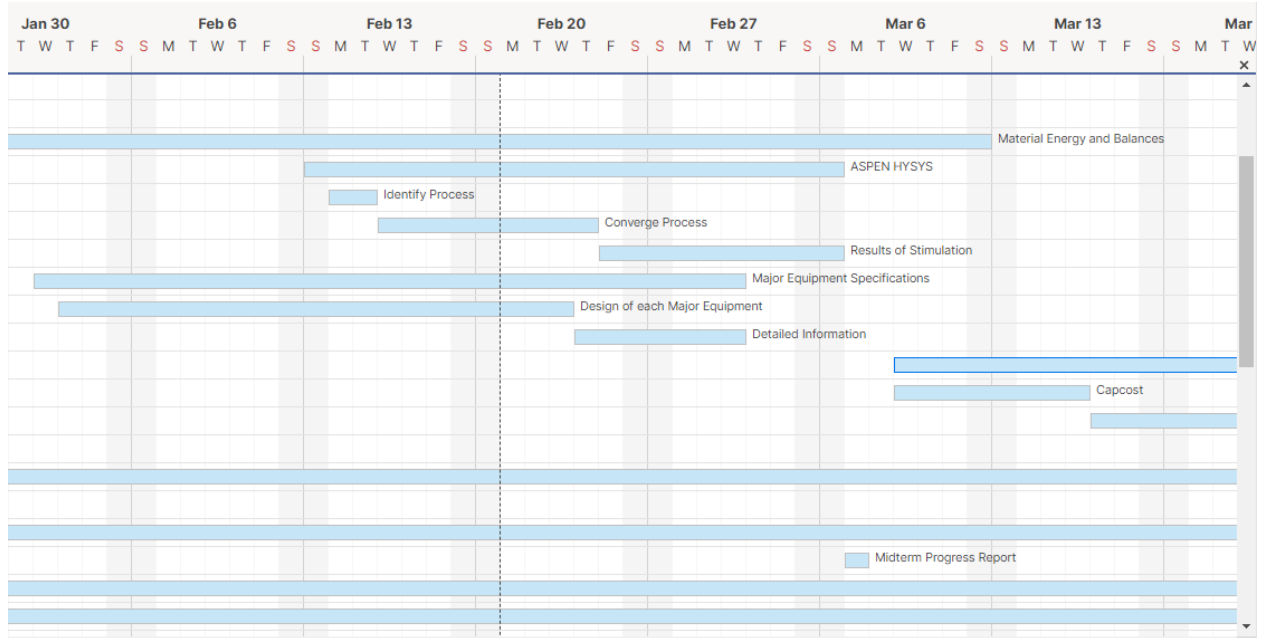
1,3 Butadiene to Ethanol Plant Design

smartsheet

Tasks	Assigned To	Duration	Start Date	End Date
Literature Search		10 days	09/21/21	10/01/21
Project Selection		2 days	09/21/21	09/22/21
Initial Research		8 days	09/23/21	10/04/21
Process Selection		9 days	10/05/21	10/15/21
Process & Reaction		8 days	10/05/21	10/14/21
Flowsheet Development		33 days	10/15/21	11/30/21
Basic Information		7 days	10/15/21	10/23/21
Process Flow Diagram Draft		21 days	10/25/21	11/22/21
Material Energy and Balances		110 days	11/22/21	03/12/22
ASPEN HYSYS		21 days	02/13/22	03/06/22
Identify Process		2 days	02/14/22	02/15/22
Converge Process		8 days	02/16/22	02/24/22
Results of Stimulation		9 days	02/25/22	03/06/22
Major Equipment Specifications		28 days	02/02/22	03/02/22
Design of each Major Equipment		21 days	02/03/22	02/23/22
Detailed Information		7 days	02/24/22	03/02/22
Economic Analysis		22 days	03/09/22	03/31/22
Capcost		7 days	03/09/22	03/16/22
Cost Evaluation		7 days	03/17/22	03/24/22
Develop Cash Flow		7 days	03/25/22	03/31/22
Reporting		207 days	09/21/21	04/16/22
Selecting Process		2 days	09/21/21	09/22/21
Homework Assignments		198 days	09/21/21	04/09/22
Midterm Progress Report		TBD	TBD	03/07/22
End of the semester Report		86 days	01/20/22	04/16/22
End of semester Presentation		86 days	01/20/22	04/16/22



✓



✓

CHEG 4248 Confidential TEAM Member Evaluation
PROJECT TITLE: Production of 1,3 butadiene from ethanol

TEAM #:1 ASSIGNMENT/HOMEWK#:1 LAST NAME:Christie FIRST NAME:Jevaun
Directions: Fill out the evaluation for EACH member of your team in the correct column. **PLEASE INCLUDE YOURSELF.** Rate the performance of each student in each category on a 5 point scale (1 - Pathetic, 2 - Poor, 3 - Fair, 4 - Good, 5 - Excellent).

Names: A: Jevaun Christie

B: Au'MyiaCollins

C. Mohammed Akinotoch

D: Cayla Alexander

E. Duaa Al Dabri

F:

Evaluation:

1. Student attended and contributed to the group meetings.

A: 5 B: 5 C: N/A D: 4 E: 2 F:

2. Student performed his/her assigned tasks in a timely manner.

A: 5 B: 5 C: N/A D: 4 E: 2 F:

3. Student performed technical tasks in a quality manner.

A: 5 B: 5 C: N/A D: 4 E: 2 F:

4. Student contributed to setting weekly goals and dates for tasks.

A: 5 B: 5 C: N/A D: 4 E: 2 F:

5. Student was willing to work toward the benefit of the group.

A: 5 B: 5 C: N/A D: 4 E: 2 F:

6. Student kept up to date with current project progress and logbook.

A: 5 B: 5 C: N/A D: 4 E: 2 F:

7. Rate the overall performance of the student as a member of the team on this project.

A: 5 B: 5 C: N/A D: 4 E: 2 F:

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I

Spring 2022

PROJECT ASSIGNMENT COVER SHEET

TEAM NUMBER: 1

ASSIGNMENT #: 1

Assignment Title: Minutes of Meeting

Due Date: 02/17/2022

No	TEAM Member Name TEAM Member Signature	Brief Description of Work Assigned to Member	% Completed by Member*	Your Score
1	Jevaun Christie	• Setting up meetings • Emailing professor	100%	100
	JC			

		Working on first portion of Homework #1 (section a and b)		
2	Au'Myia Collins	- Working on second portion of Homework #1 (section b and c) - Making sure document was sufficient before turning in assignment - Contributed to arranging group meetings	100%	100
	AC			
3	Mohammed Akinotcho	- Providing the Gantt chart(section f) - Making sure document was sufficient before turning in assignment	N/A	N/A
	MA			
4	Cayla Alexander	- Formatting Homework #1 - Working on section e	100%	100
	CA			
5	Duaa Al Badri	- Formatting Homework #1 - Working on section d	70%	70
	DB			

By signing this assignment cover sheet, I agree that the percentages stated in the % completed column reflect the contribution made by me and other members of the group.

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I

FALL 2021

MINUTES OF TEAM MEETINGS

Meeting Date(s): Feb. 3, 10, & 17 Meeting Time: Varies Meetings Location: In Person

Members Present: Jevaun Christie, Au'Myia Collins, Mohammed Akinotcho,

Cayla Alexander, Duaa Al Badri

Agenda for Meeting (List all items to be discussed or discussed at the meeting)

- Distribute workload for homework 1
- Work on ASPEN HYSYS
- Designing of Major Equipment

Detailed Minutes: (should include name of speaker and summary of what he/she suggested)

Jevaun Christie: Developed plan of distributing workload for homework 1, expressed strong suit in ASPEN HYSYS, explained previous knowledge of ethanol

Au'Myia Collins: Conducting zoom meetings 1-2 times for the week, has great experience with mass balance equations, mentioning previous background knowledge of ethanol, expressed different thoughts on how to plan accordingly when completing work, etc.

Cayla Alexander: Completed Gantt Chart

Mohammed Akinotcho: Has experience in Gantt charts building, kindly expressed his expertise in multiple areas, and made sure homework formatting was set up correctly. Expressed his situation but will be back soon.

Duaa Al Badri: N/A

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I

FALL 2021

TASK ASSIGNMENT & DELIVERABLES AT MEETINGS

Use this table to document tasks assigned and deliverables completed/submitted by each group member at each meeting. If deliverables are not completed, indicate the actions taken by the group on this individual.

Meeting Date: Feb. 3, 10, & 17 Meeting Time: Varies Meeting Location: In-Person

Name	Task Assigned	Deliverables Completed and Submitted
Jevaun Christie	• Setting up meeting • Emailing professor • Working on first portion of Homework #1 (section a and b)	Yes; Yes

Au'Myia Collins	• Working on second portion of Homework #1 (section b and c) • Making sure document was sufficient before turning in assignment • Contributed to arranging group meetings	Yes; Yes
Mohammed Akinotcho	• Providing the Gantt chart (section f) • Making sure document was sufficient before turning in assignment	N/A; N/A
Cayla Alexander	• Formatting Homework #1 • Assigned to section e	Yes; Yes
Duaa Al Badri	• Formatting Homework #1 • Assigned to section d	No; No

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I

FALL 2021

CLASS ATTENDANCE SHEET

2
OK

This table documents attendance of students of the Senior Design & Professionalism class as indicated below and will be used to evaluate the sub outcome of ABET criterion 4 Students understanding and demonstration of professional responsibilities.

Meeting Date: Feb. 3, 10, & 17 Meeting Time: Varies Meeting Location: In-Person

Student Name	Project Title	On time	5 minutes late	Absent
Jevaun Christie	Production of 1,3 Butadiene from ethanol	Yes	No	No
Au'Myia Collins	Production of 1,3 Butadiene from ethanol	Yes	No	No
Mohammed Akinotcho	Production of 1,3 Butadiene from ethanol	N/A	No	No
Cayla Alexander	Production of 1,3 Butadiene from ethanol	Yes	No	No

Duaa Al Badri	Production of 1,3 Butadiene from ethanol	Only attended zoom meeting (did not speak/ input ideas)	No	Absent to all in person meetings

BELOW AVERAGE

Below Average Student Original Graded Assignment on Home Work 1

Prairie View A&M University

Roy G. Perry College of Engineering Department:

Spring 2022



✓ OK

80%

Chemical Engineering CHEG 4247-P01

Senior Design & Professionalism

Homework #1

Date Due: February 17, 2022

Submitted by:

Team #4: Taylon Owens, Amiya Rogers, Cinthia Sahin, Laura Ukpede

Submitted to: Dr. Emmanuel Dada

CHEG 4247 - Senior Design & Professionalism I (Fall 2021):

Homework 1

February 15, 2022

Due: February 17, 2022

You will be graded based on your ability to define and plan the project. Clarity of presentation is essential if you are to avoid losing points.

- (a) Create a list of major tasks and their respective duration to be accomplished to enable you achieve the goals and objectives for your project**
- (b) Organize the tasks into phases/module**
- (c) Identify sub-tasks and their respective duration**
- (d) Link major tasks and/or sub-tasks when required**
- (e) Identify milestones and deadlines to track an important event**
- (f) Prepare a Gantt Chart and print it out using Microsoft Project or Excel**

**DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM II CHEG 4248
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR SPRING 2022 SEMESTER**

ABET Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.

Assignments that test competency in this area will include problems that test a student's ability to (1) accommodate the needs of others, (2) share responsibilities, (3) commit to team goals, (4) apply principles of constructive conflict management to interaction with others, (5) support members, and (6) communicate with team members.

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Max for this Assignment	Your Score
Outcome 5: An ability to function effectively on a team whose members together, provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.		
Ability to follow good team management practices and resolving conflicts <i>Plan group meetings and time management, distribute project tasks evenly,.</i>	50	48
An ability to track and meet project schedule <i>Evaluate performance of team members on a regular basis, and track progress of team members</i>	50	32
TOTAL	100	80

(a) Create a list of major tasks and their respective duration to be accomplished to enable you to achieve the goals and objectives for your project

Task	Duration
1. HYSYS/ASPEN Simulation of Process	1 week
2. Chemical Engineering Design	4 weeks
3. Economic Evaluation	2 weeks
4. Safety and HAZOP Analysis	2 weeks
5. Finish Report	1 week
6. Visual & Oral Presentation	1week

(b) Organize the tasks into phases/module

PHASE 1: Steps 1-2

PHASE 2: Steps 3-4

PHASE 3: Steps 5-6

(c) Identify sub-tasks and their respective duration

Phase	Task	Sub-task	Duration
1	1. HYSYS/ASPEN Simulation Process	Include Small Equipment	1 week
		Verify Recycle Stream	1 week
		Converge	1 week
	2. Chemical Engineering Design	Design of Major Equipment	4 weeks
		Detailed Unit P&ID (Reactor)	4 weeks
		Listing Equipment and Specification	4 weeks
2	3. Economic Evaluation	Cost of Major Equipment Using CAPCOST Software	2 weeks
		Fixed Capital Costs	2 weeks
		Utilities	2 weeks
		Fixed Capital Investment	2 weeks
		Manufacturing Production Costs	2 weeks
		Peters and Timmerhaus Software	2 weeks
		Complete Economic Analysis	2 weeks
	4. Safety and HAZOP Analysis	Methanol Safety/Hazards	2 weeks
		Reactor & Catalyst Safety/Hazards	2 weeks
		DME Safety/Hazards	2 weeks
		Specific Unit Breakdown (Distillation)	2 weeks

3	5. Finish Report	Startup/Shutdown HAZOP	2 weeks
		Complete Rough Draft	1 week
	6. Visual and Oral Presentation	Complete Final Draft	1 week
		Complete Presentation	1 week
		Presentation Practice	1 week

(d) Link major tasks and/or sub-tasks when required

The linkage of tasks and sub-tasks has been presented in the table in the Gantt Chart

(e) Identify milestones and deadlines to track an important event

There are various project milestones to ensure that the project is completed within the stipulated timeframe. These milestones are presented as follows.

Milestone	Deadline
1. HYSYS/ASPEN Simulation Process	February 25, 2022
2. Chemical Engineering Equipment Design	March 28, 2022
3. Economic Evaluation	April 13, 2022
4. Safety and HAZOP Analysis	April 13, 2022
5. Complete Final Report and Presentation	April 16, 2022
6. Final Senior Design Presentation	April 23, 2022

(f) Prepare a Gantt Chart and print it out using Microsoft Project or Excel

Please find attached the Gantt Chart

PROJECT TITLE:		PRODUCTION OF DIMETHYL ETHER (DME)																																																																	
Project start		2/18/22																																																																	
Display Week		0																																																																	
TASKS AND SUB-TASKS				OWNER		START DATE		END DATE		DURATION																																																									
DMS/ASSTEN DISCUSSION ON																																																																			
Include Small Equipment				All		18-Feb-22		25-Feb-22		1 week																																																									
Verify Recycle Stream				All		18-Feb-22		25-Feb-22		1 week																																																									
Converge				All		18-Feb-22		25-Feb-22		1 week																																																									
Design of Major Equipment				All		18-Feb-22		25-Feb-22		1 week																																																									
Listing Equipment and Specification				All		18-Feb-22		25-Feb-22		1 week																																																									
Chemical Engineering Design																																																																			
Design of Major Equipment				All		28-Feb-22		28-Mar-22		4 weeks																																																									
Detailed Unit P&ID (Reactor)				Taylor & Amiya		28-Feb-22		28-Mar-22		4 weeks																																																									
Listing Equipment and Specification				Laura & Cinthia		28-Feb-22		28-Mar-22		4 weeks																																																									
Economic Evaluation																																																																			
Cost of Major Equipment Using CAPCOST Software				Cinthia and Laura		30-Mar-22		13-Apr-22		2 weeks																																																									
Fixed Capital Costs				Taylor		30-Mar-22		13-Apr-22		2 weeks																																																									
Utilities				Taylor		30-Mar-22		13-Apr-22		2 weeks																																																									
Fixed Capital investments				Taylor		30-Mar-22		13-Apr-22		2 weeks																																																									
Manufacturing Production costs PETERS and Timmerhaus				Amiya		30-Mar-22		13-Apr-22		2 weeks																																																									
Complete Economic Analysis/ Cash Flow Diagram				All		30-Mar-22		13-Apr-22		2 weeks																																																									
Safety and HAZOP Analysis																																																																			
Methanol Safety/Hazards				Laura		30-Mar-22		13-Apr-22		2 weeks																																																									
Reactor & Catalyst Safety/Hazards				Taylor		30-Mar-22		13-Apr-22		2 weeks																																																									
DME Safety/Hazards				Amiya		30-Mar-22		13-Apr-22		2 weeks																																																									
Specific Unit Breakdown (Distillation)				Cinthia		30-Mar-22		13-Apr-22		2 weeks																																																									
Startup/Shutdown HAZOP				Amiya		30-Mar-22		13-Apr-22		2 weeks																																																									
Finish Report																																																																			
Complete Rough Draft				All		9-Apr-22		16-Apr-22		1 week																																																									
Complete Final Draft				All		9-Apr-22		16-Apr-22		1 week																																																									
Visual & Oral Presentation																																																																			
Complete Presentation				All		9-Apr-22		16-Apr-22		1 week																																																									
Presentation Practice				All		9-Apr-22		16-Apr-22		1 week																																																									

CHEG 4248 Confidential TEAM Member Evaluation

PROJECT TITLE:

TEAM #: 4 ASSIGNMENT/HOMEWK#: 1 LAST NAME: Rogers FIRST NAME: Amiya
Directions: Fill out the evaluation for EACH member of your team in the correct column. **PLEASE INCLUDE YOURSELF.** Rate the performance of each student in each category on a 5 point scale (1 – Pathetic, 2 – Poor, 3 – Fair, 4 – Good, 5 – Excellent).

Names: A: Amiya Rogers B: Taylon Owens

C: Cinthia Sahin D: Laura Nkpede

E: N/A F: N/A

Evaluation:

1. Student attended and contributed to the group meetings.

A: 5 B: 5 C: 5 D: 5 E: — F: —

2. Student performed his/her assigned tasks in a timely manner.

A: 5 B: 5 C: 5 D: 5 E: — F: —

3. Student performed technical tasks in a quality manner.

A: 5 B: 5 C: 5 D: 5 E: — F: —

4. Student contributed to setting weekly goals and dates for tasks.

A: 5 B: 5 C: 5 D: 5 E: - F: -

5. Student was willing to work toward the benefit of the group.

A: 5 B: 5 C: 5 D: 5 E: - F: -

6. Student kept up to date with current project progress and logbook.

A: 5 B: 5 C: 5 D: 5 E: - F: -

7. Rate the overall performance of the student as a member of the team on this project.

A: 5 B: 5 C: 5 D: 5 E: - F: -

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I FALL 2021 PROJECT ASSIGNMENT COVER SHEET

TEAM NUMBER Dada Team 4

ASSIGNMENT # HWK 1

Assignment Title: HWK 1

Due Date: February 17, 2022

No	TEAM Member Name TEAM Member Signature	Brief Description of Work Assigned to Member	% Completed by Member*	Your Score
1	Taylon Owens	Complete tasks assigned in homework #1	100%	
2	Amiya Rogers	Complete tasks assigned in homework #1	100%	
3	Laura Ukpede	Complete tasks assigned in homework #1	100%	
4	Cinthia Sahin	Complete tasks assigned in homework #1	100%	
5				

*100% means the member completed his/her assigned work.

By signing this assignment cover sheet, I agree that the percentages stated in the % completed column reflect the contribution made by me and other members of the group.

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I FALL 2021

MINUTES OF TEAM MEETINGS

Meeting Date: February 14, 2022 Meeting Time: 11:30 AM Meeting Location: Face to Face

Members Present: Taylon Owens, Amiya Zhanee Rogers, Laura O Ukpede, and Cinthia Yohana Sahin

Agenda for Meeting

We got together as a team and discussed homework 1 assignment. We discussed and finished components A, B, and C of the homework. Lastly, we set up a follow up date and time to finish parts D, E, and F of the homework one assignment.

Detailed Minutes: (should include name of speaker and summary of what he/she suggested)

- **Taylon Owens-** Identified major tasks regarding overall completion of the design project.
- **Amiya Rogers-** Suggested major tasks and numerous subtasks for the homework.
- **Laura O Ukpede-** Helped with subtasks and tasks for the homework.
- **Cinthia Sahin-** Contributed to the subtasks and time duration for each task.

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I FALL 2021

TASK ASSIGNMENT & DELIVERABLES AT MEETINGS

Use this table to document task assigned and deliverables completed/submitted by each group member at each meeting. If deliverables are not completed, indicate the actions taken by the group on this individual

Meeting Date:February 14, 2022 Meeting Time:11:30 AM Meeting Location: Face to Face

Name	Task Assigned	Deliverables Completed & Submitted
Amiya Rogers	A, B, C	Completed tasks A, B, C
Cinthia Sahin	A, B, C	Completed tasks A, B, C
Taylon Owens	A, B, C	Completed tasks A, B, C
Laura Ukpede	A, B, C	Completed tasks A, B, C

CHEG 4247 SENIOR DESIGN AND PROFESSIONALISM I

FALL 2021

CLASS ATTENDANCE SHEET

This table documents attendance of students of the Senior Design & Professionalism class as indicated below and will be used to evaluate the sub outcome of ABET criterion 4 Students understanding and demonstration of professional responsibilities.

Meeting Date: February 14, 2022 Meeting Time: 11:30AM Meeting Location: Face to Face

Student Name	Project Title	On time	5 minutes late	Absent
Amiya Rogers	Production of Dimethyl Ether	X		
Taylon Owens	Production of Dimethyl Ether	X		
Laura Ukpede	Production of Dimethyl Ether	X		
Cynthia Sahin	Production of Dimethyl Ether	X		

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