

Production of 1,3 Butadiene From Ethanol



JAM CHEMICAL
• CHEMICAL PLANT •

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Senior Design I

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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

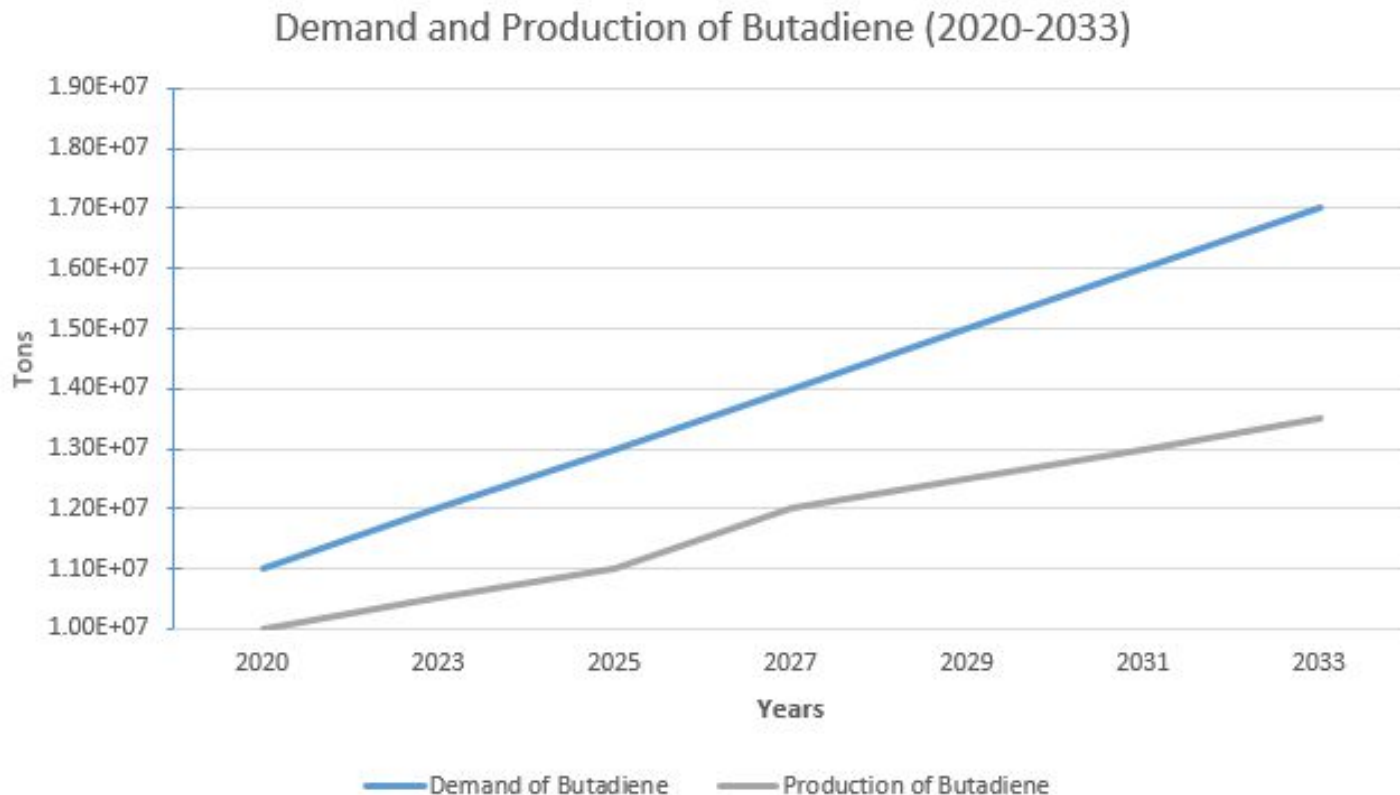
(Capacity & Location)

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

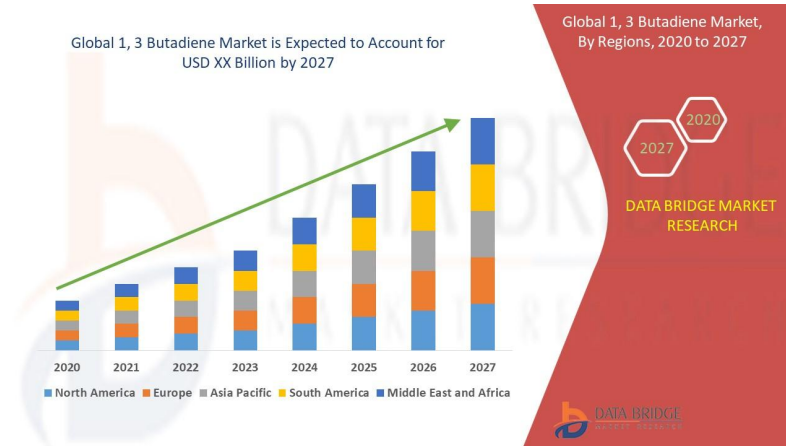
- Close to large body of water
- Nearby Interstate Grain Corporation deep water export facility and ADM deep water export facility
- Transportation of Raw Materials:
 - Railroad
 - Ocean Vessels
 - Tanker Trucks



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

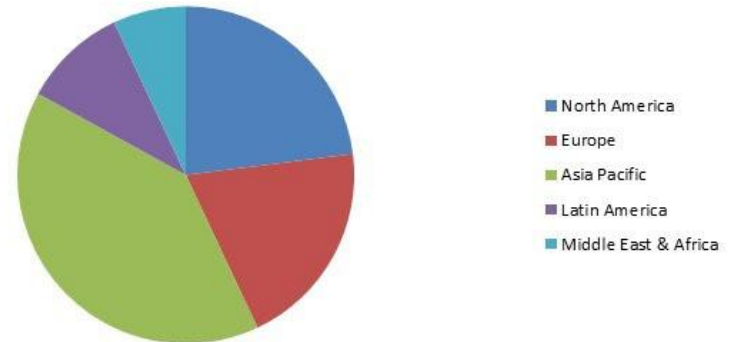


MARKET ANALYSIS

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

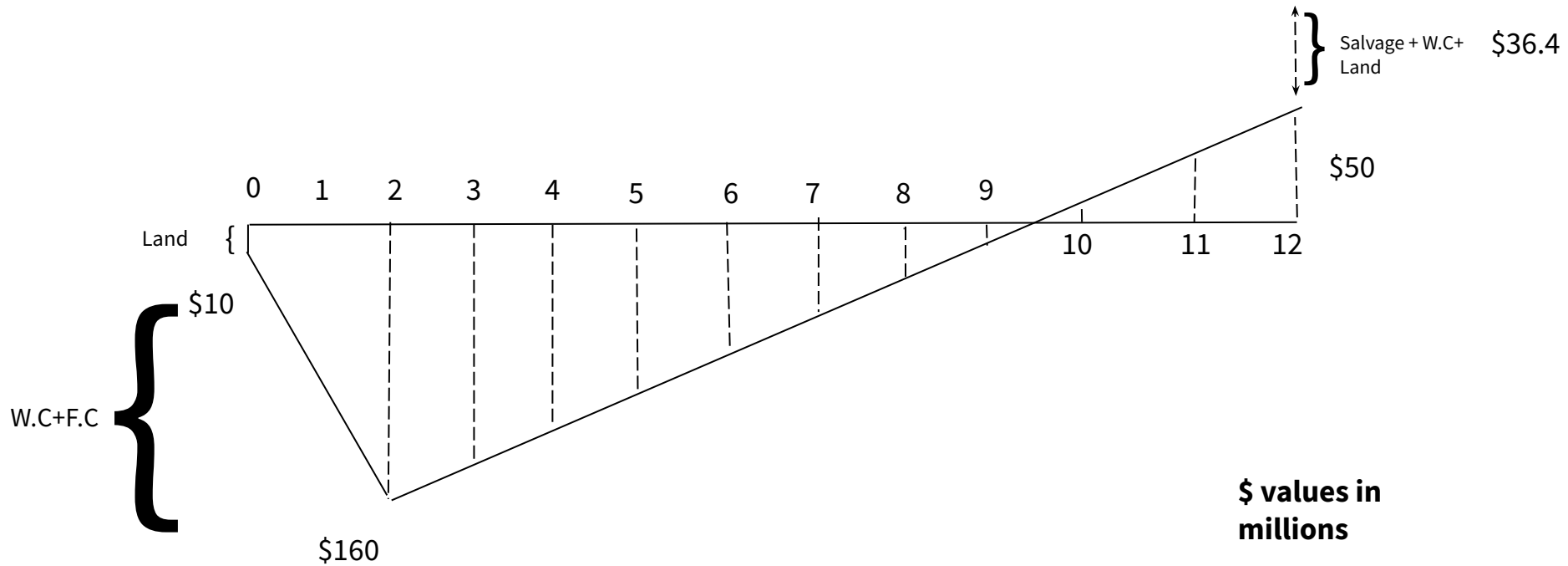


Firestone



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

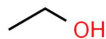
PRODUCTION ROUTES	PROS	CONS
Extraction from C4 hydrocarbons	Cheap raw material	High operating cost Low selectivity Non sustainable Toxic
Dehydrogenation of n-butane	Cheap raw material	Low selectivity Less sustainable
Ethanol ✓	Cheap raw material Non toxic Biorenewable Environmental Friendly	Endothermic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

ONE STEP PROCESS VS TWO STEP PROCESS

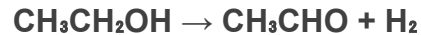
PROCESSES	PROS	CONS
ONE STEP (IPATIEV Process)	Low complexity reactions	Higher capital costs due to multiple reactors
TWO STEP (OSTROMYSLENSKY) Process ✓	Higher % Yield (18%) 98% Purity Less energy consumed due to lower reaction temperature	Limited process optimization High Energy consumption

PROCESS CHEMISTRY

Chemical structures/ information about each compound

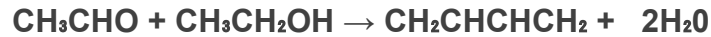
	Ethanol	Acetaldehyde	Hydrogen Gas	1,3 Butadiene	Water
Molecular Weight	0.1016lbs/mol	0.097 lbs/mol	2.016 lb/lbmol	54.09 lb/lbmol	0.040 lbs/mol
Chemical Formula	C ₂ H ₆ O	C ₂ H ₄ O	H ₂	CH ₂ CHCHCH ₂	H ₂ O
Chemical Structure					
Boiling Point	78.39°C (173.1°F)	20.2°C (68.36°F)	-252.89°C (-423.2°F)	-4.4°C (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.

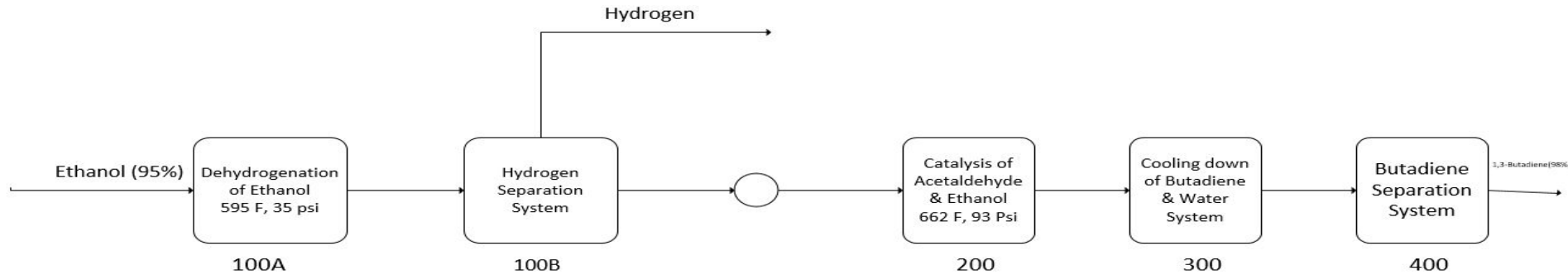
PROCESS CHEMISTRY



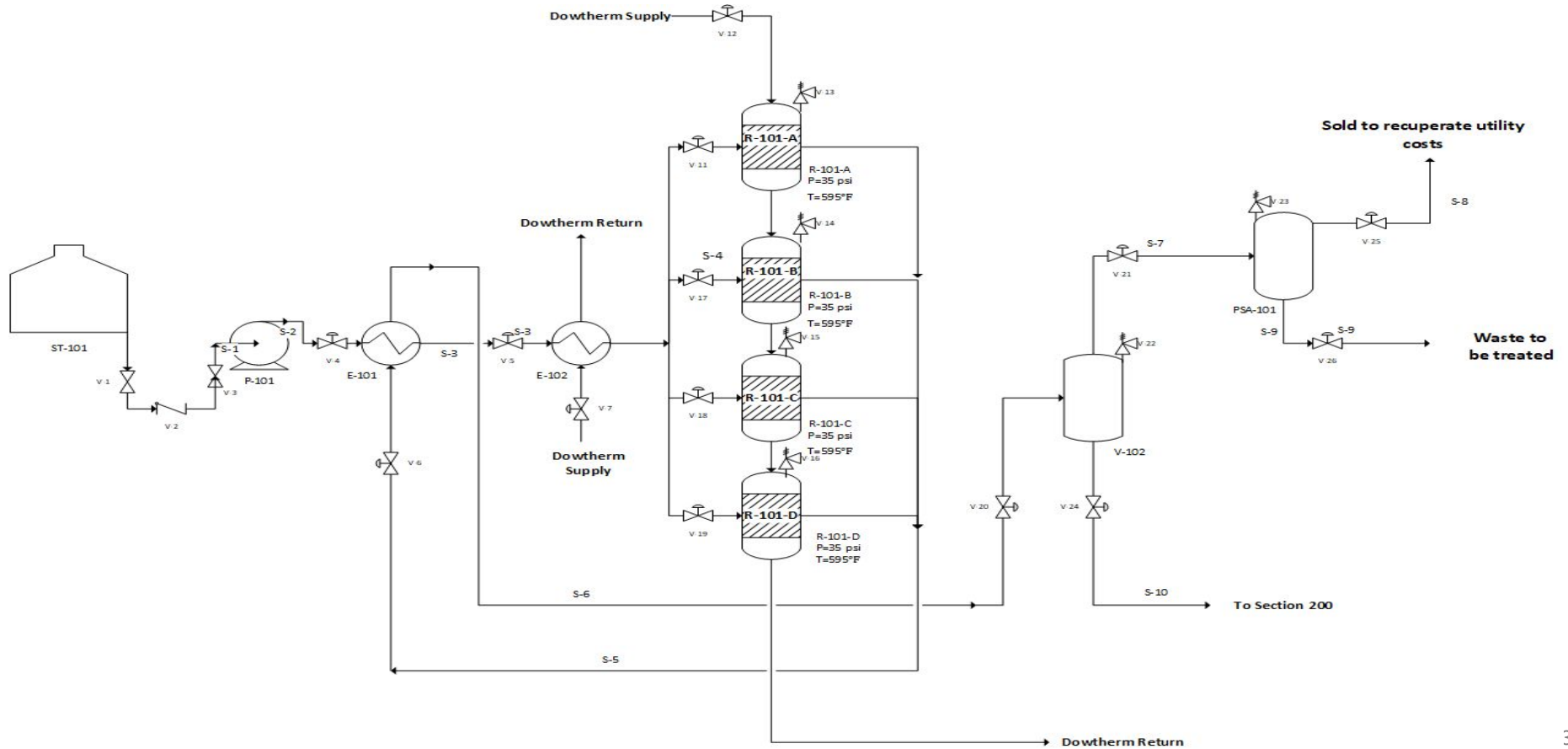
- ❑ In the second step of the Process Acetaldehyde is mixed with ethanol to form butadiene and water in a heterogeneous tantalum-silica catalyst with 55% selectivity on same type of reactor as the first reaction.
- ❑ Finally, this last product goes through a distillation train to separate our final product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

PROCESS FLOW DIAGRAM

BLOCK FLOW DIAGRAM



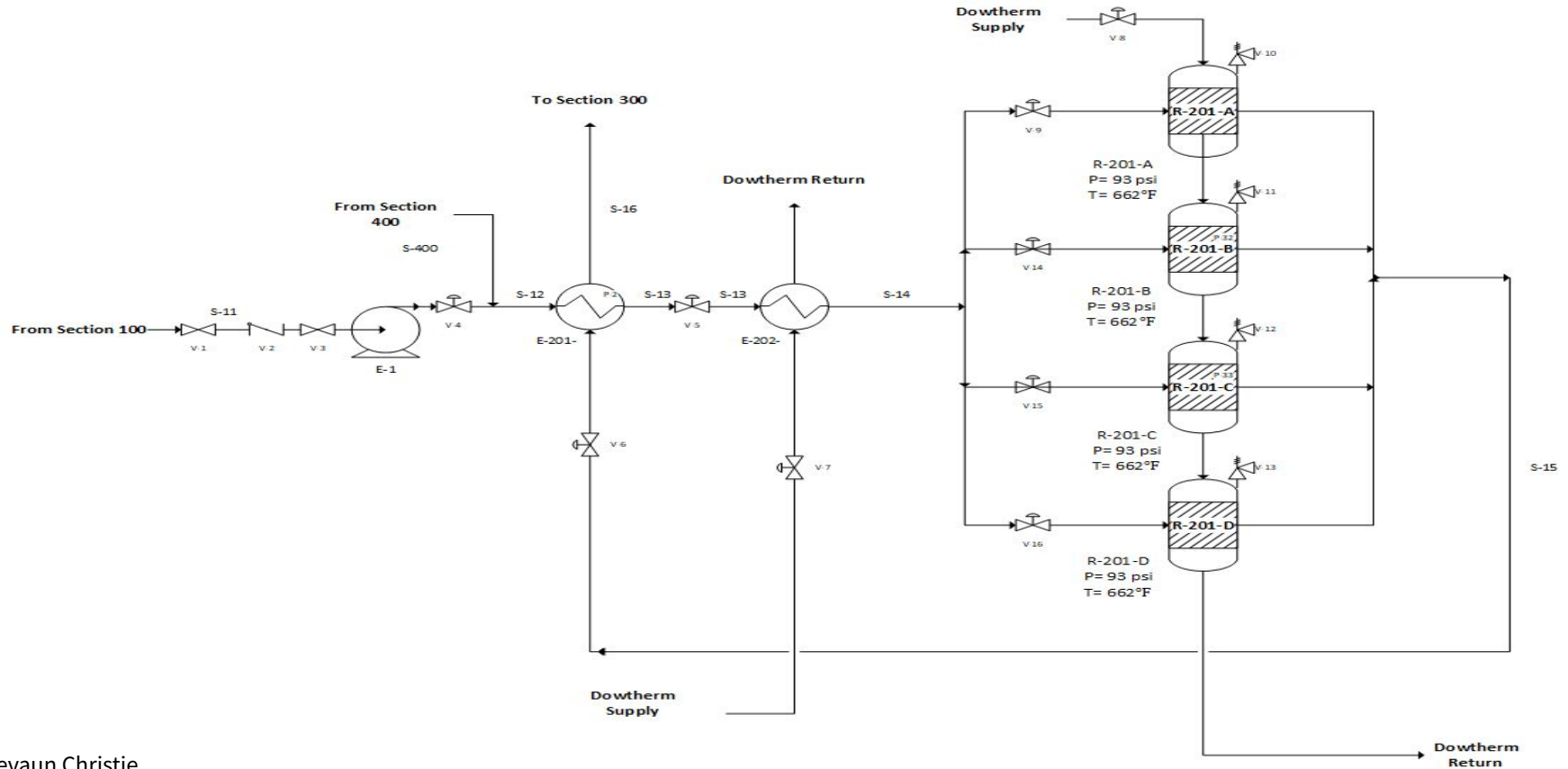
SECTION 100



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

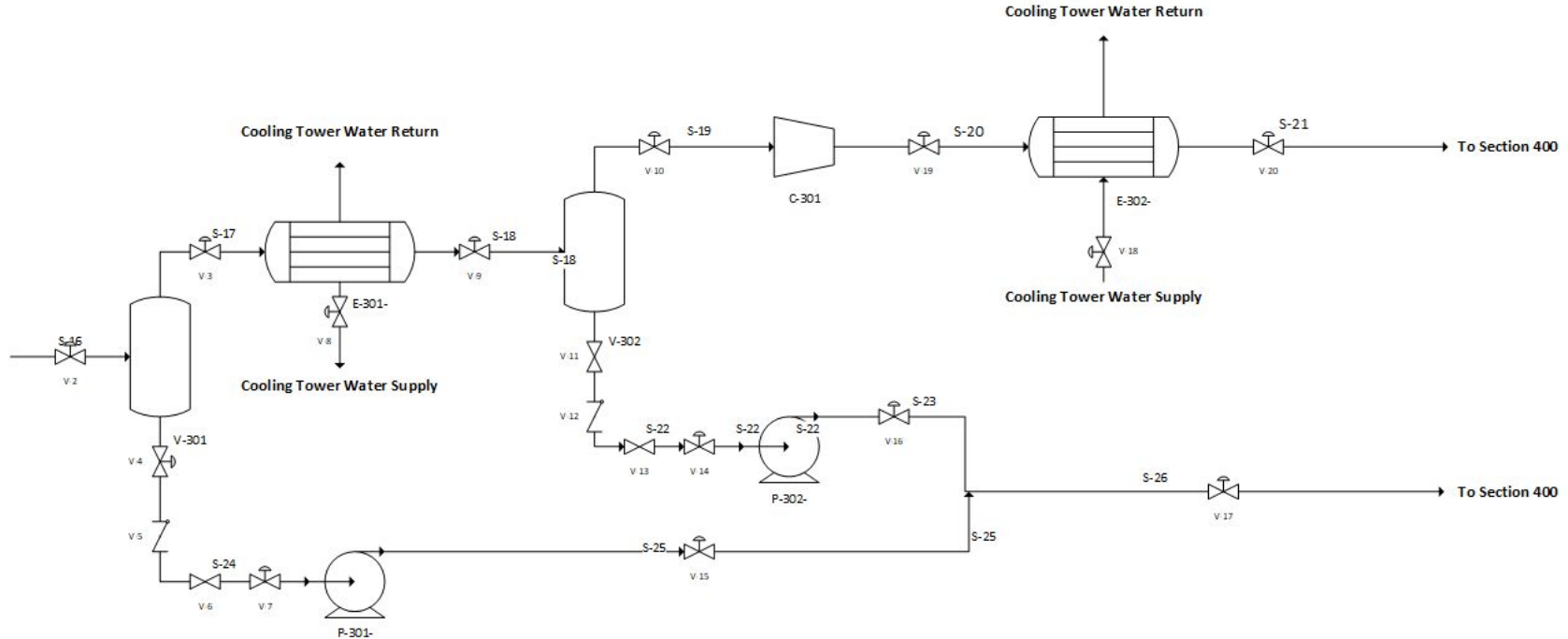
SECTION 200



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

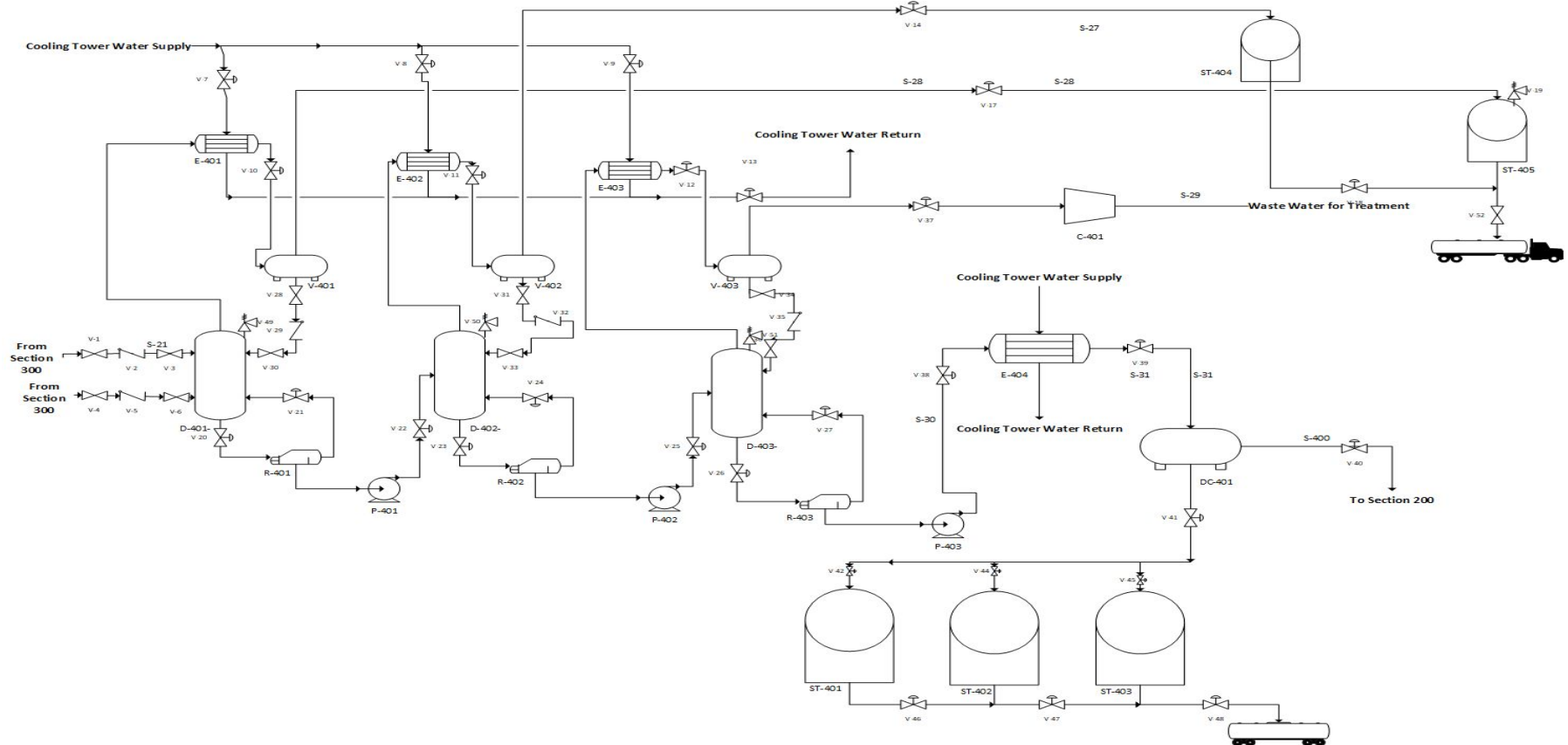
SECTION 300



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	

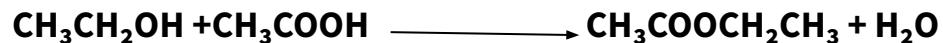
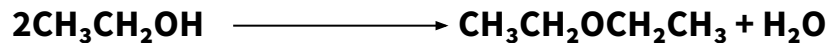
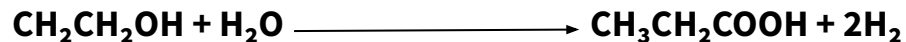
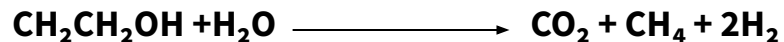
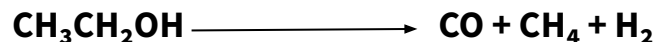
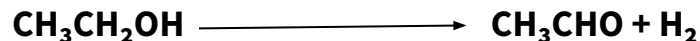
MATERIAL BALANCE FOR THE SECOND REACTOR

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

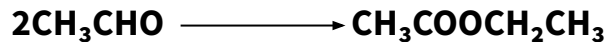
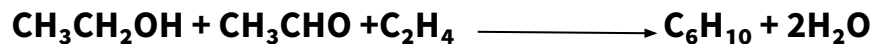
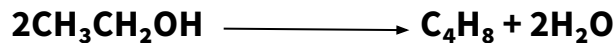
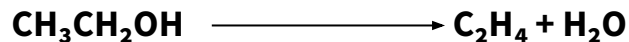
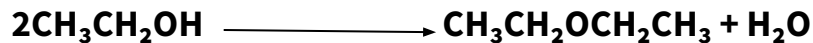
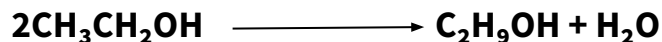
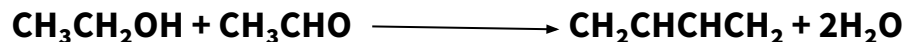
❖ Ethyl Acetate

❖ 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

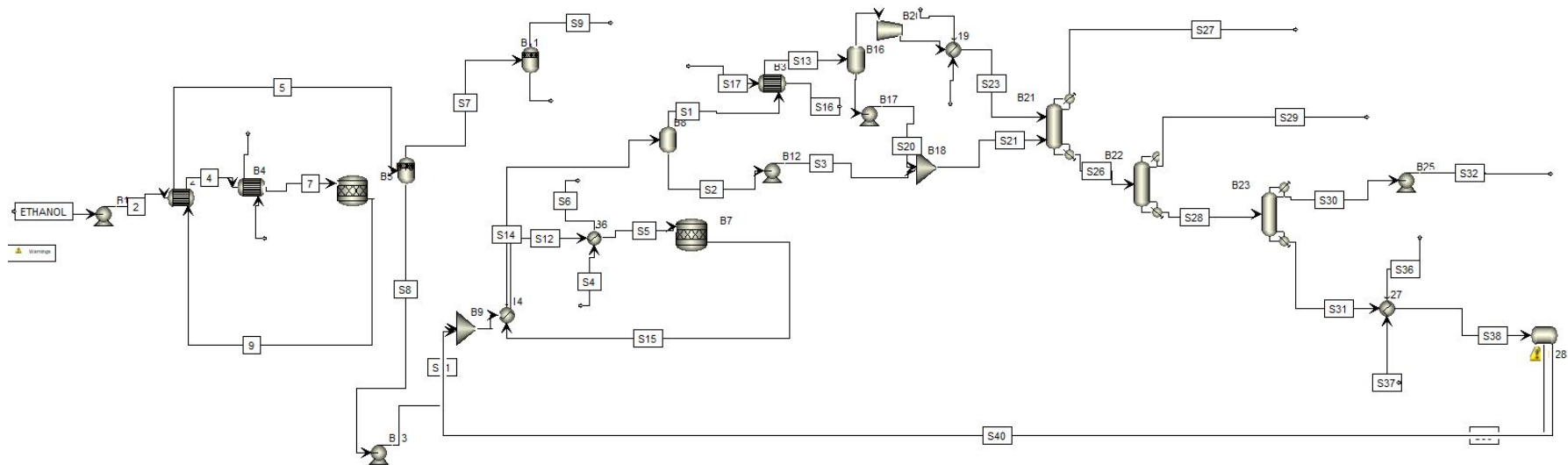
Multi-Stage Compressor	MSC-201	-60 MMBTU/hr to cool S9 from 152 °F to 107 °F	Cooling Water
Heat Exchanger	E-401	-30 MMBTU/hr to cool S28 from 231 °F to 200 °F	Cooling Water
Heat Exchanger	E-402	-20 MMBTU/hr to cool S31 from 281 °F to 200 °F	Cooling Water
Heat Exchanger	E-403	-78 MMBTU/hr to condense 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

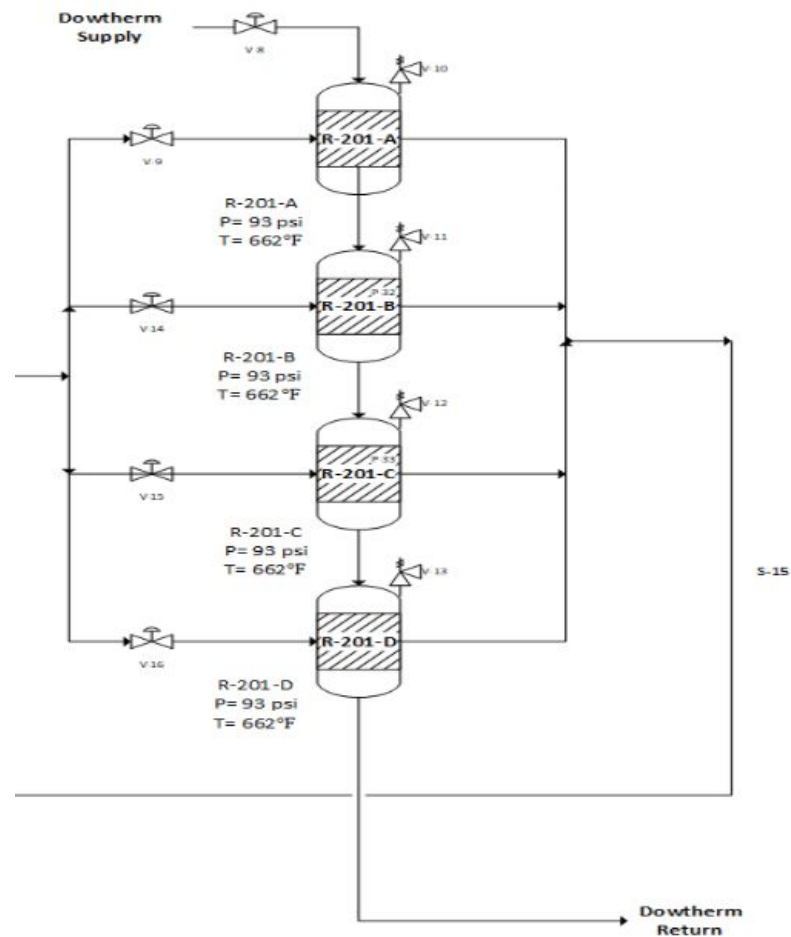
ASPEN SIMULATION



SPECIFICATION SHEET

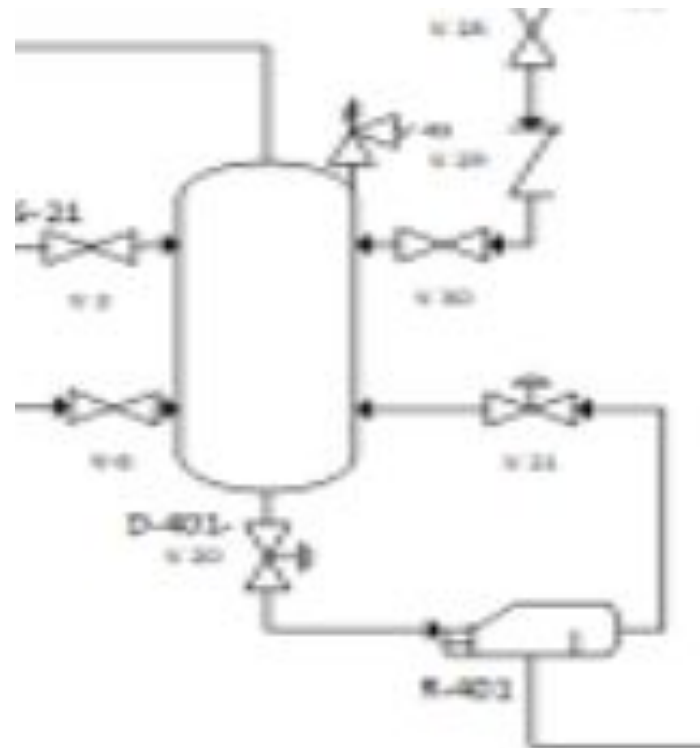
Shell and Tube Packed Bed Reactor

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



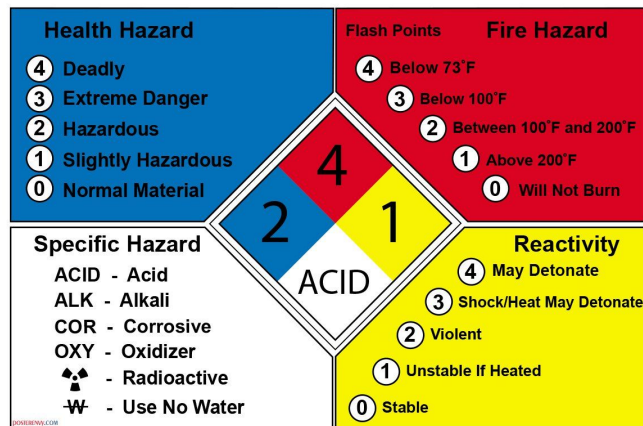
Butadiene

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)

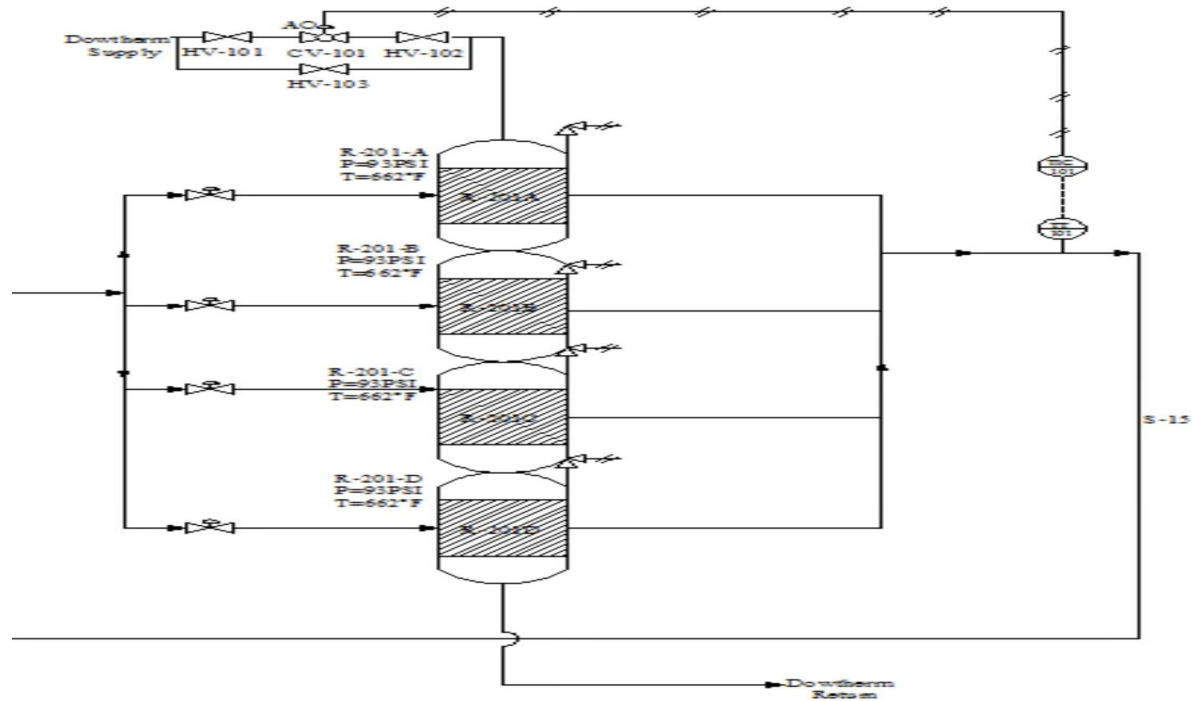
HANDLING

- ❑ 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

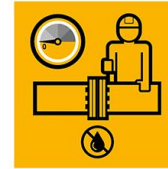
The health effects caused by exposure to 1,3-butadiene can be under two categories

- Acute exposure
- Chronic effect

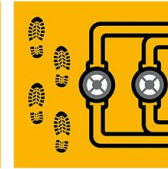
1,3 butadiene is on Hazardous substance

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



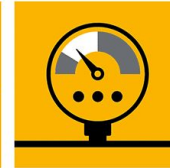
Control ignition sources



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: $V_{catalyst} = N_t \cdot Volumetric\ flowrate_{one\ tube}$
- Tube side pressure drop:

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

- Shell Diameter: $D_S = \sqrt{\left(\frac{N_t}{3} \cdot (square\ pitch)^2 \cdot \frac{4}{\pi}\right)} + 2 \cdot tube\ outer\ diameter + 1$
- Heat transfer coefficient: $U = \frac{Q}{A \cdot \Delta T}$

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

CONVERSION CHART

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: copy from values at left or	Calculated values, million \$
	Solid-processin g plant	Solid-fluid processin g plant	Fluid processin g plant		

Direct Costs

Purchased equipment, E'					24,000
Delivery, fraction of E'	0.10	0.10	0.10	0.10	2,400
Subtotal: delivered					26,400
Purchased equipment	0.45	0.39	0.47	0.47	12,408
Instrumentation&Controls(ins	0.18	0.26	0.36	0.36	9,504
Piping (installed)	0.16	0.31	0.68	0.68	17,952
Electrical systems (installed)	0.10	0.10	0.11	0.11	2,904
Buildings (including services)	0.25	0.29	0.18	0.18	4,752
Yard improvements	0.15	0.12	0.10	0.10	2,640
Service facilities (installed)	0.40	0.55	0.70	0.70	18,480
Total direct costs	1.69	2.02	2.60	2.60	35,040

Indirect Costs

Engineering and supervision	0.33	0.32	0.33	0.33	8,712
Construction expenses	0.39	0.34	0.41	0.41	10,824
Legal expenses	0.04	0.04	0.04	0.04	1,056
Contractor's fee	0.17	0.19	0.22	0.22	5,808
Contingency	0.35	0.37	0.44	0.44	11,616
Total indirect costs	1.28	1.26	1.44	1.44	38,016

Fixed capital investment (FCI)

133,056

Scale "Evaluation" and
"Year-0 \$", then
adjusted as described below

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

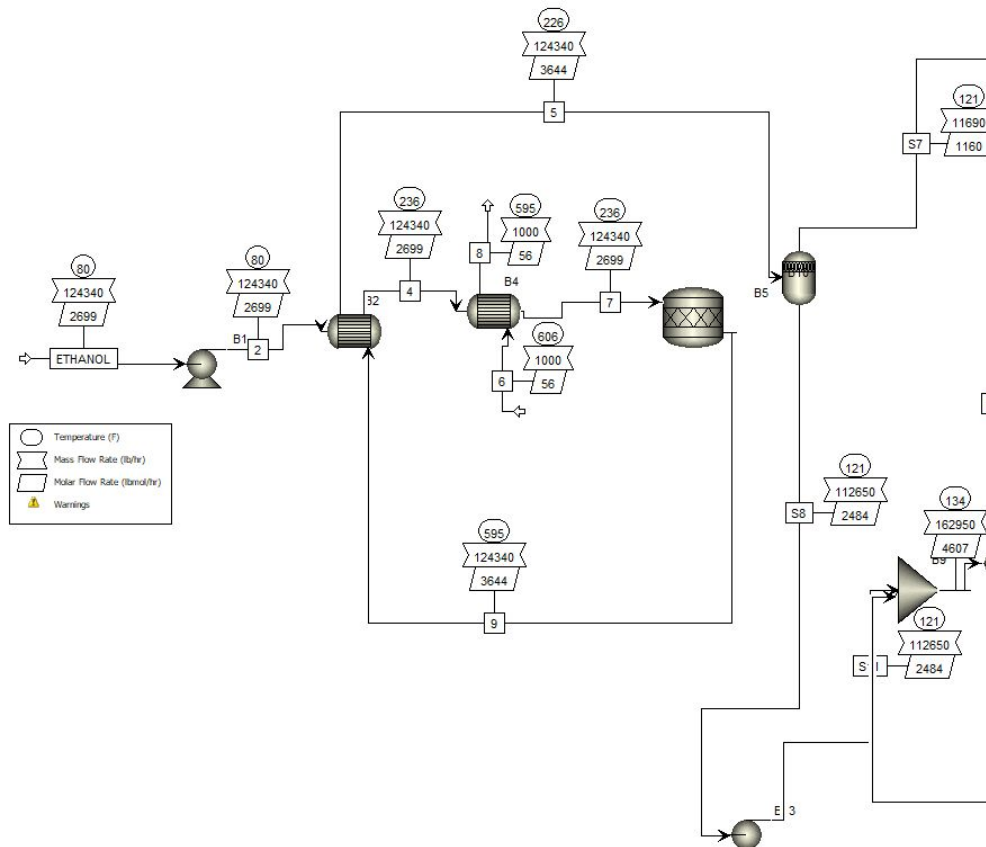
RESULT			
Products, Coproducts and Byproducts			
Name of Material	Price, \$/kg	Annual Amount, million kg/y	Annual value of product, million \$/y
1,3 BD	2.20	182.000	400.40
H2	3.25	10.700	34.78
			0.00
			0.00
			0.00
			0.00
Total annual value of products =			435.18
			Sent to 'Evaluation' and 'Year-0 \$'

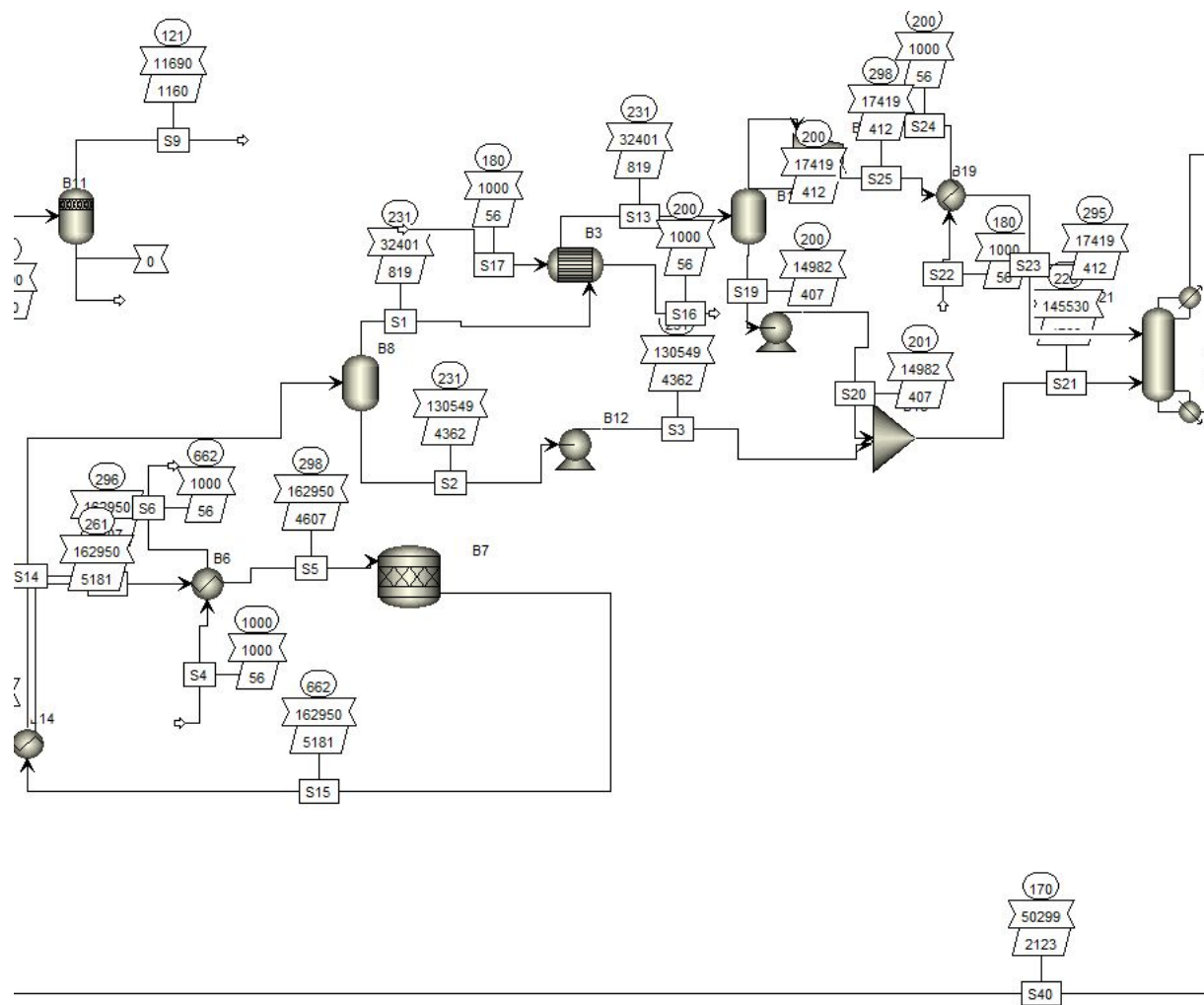
Raw Materials			
Name of Material	Price, \$/kg	Annual Amount, million kg/y	Annual raw materials cost,
1	0.73	525.000	383.25
			0.00
			0.00
			0.00
Total annual cost of raw materials =			383.25
			Sent to sheet

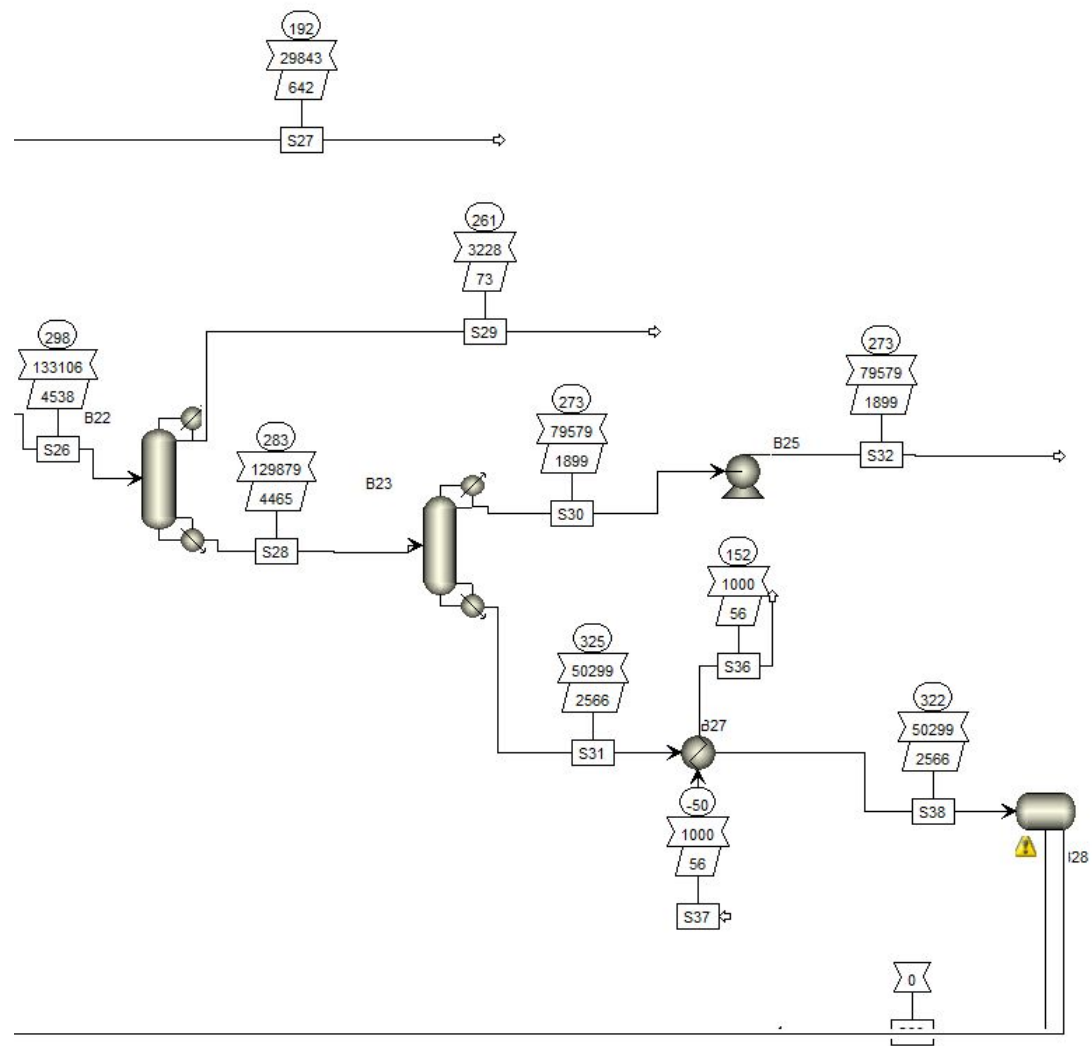
RESULT			
Operating Labor			
Number of operators per shift*	Shifts per day**	Operator rate, \$/h #	Annual operating labor cost,
8	3	33.67	2,360
*See Tables 6-13 and Fig. 6-9.			
**Default = 3 for continuous process.			
Enter appropriate value for batch operation.			
#To obtain current, local value, enter (latest local ENR skilled labor index)/6067 =			
			1

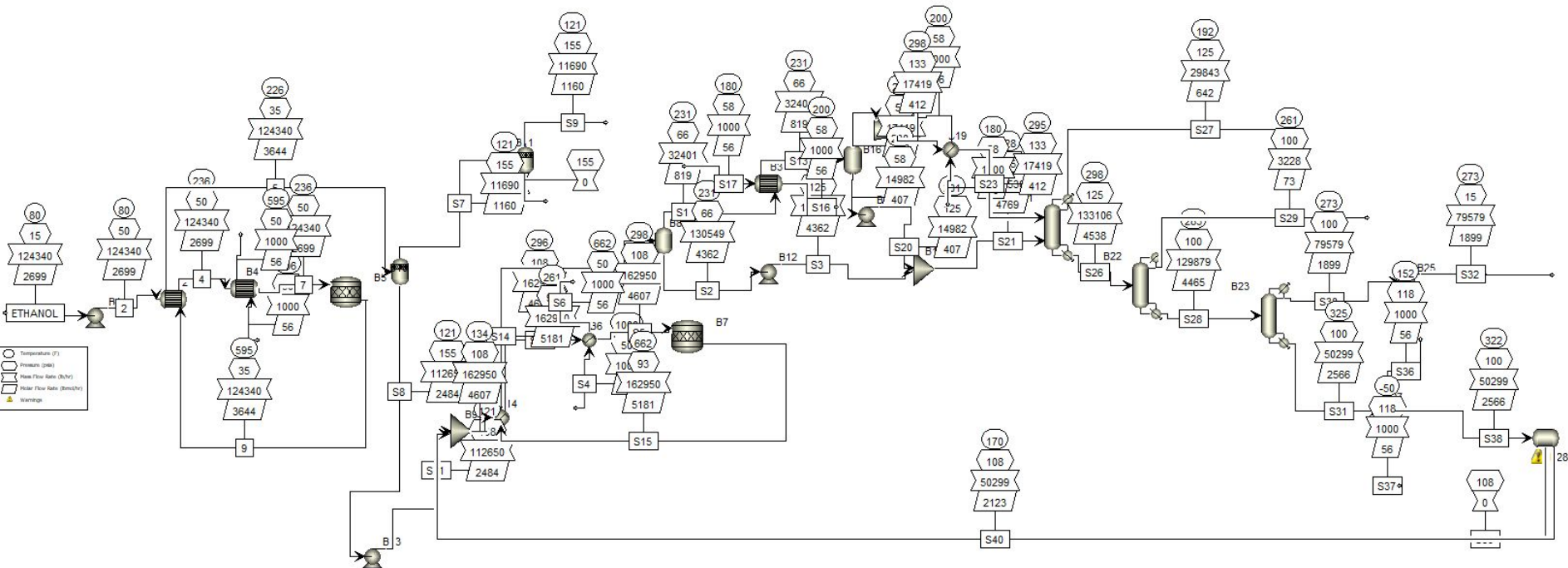
Sent to 'Annual TPC'

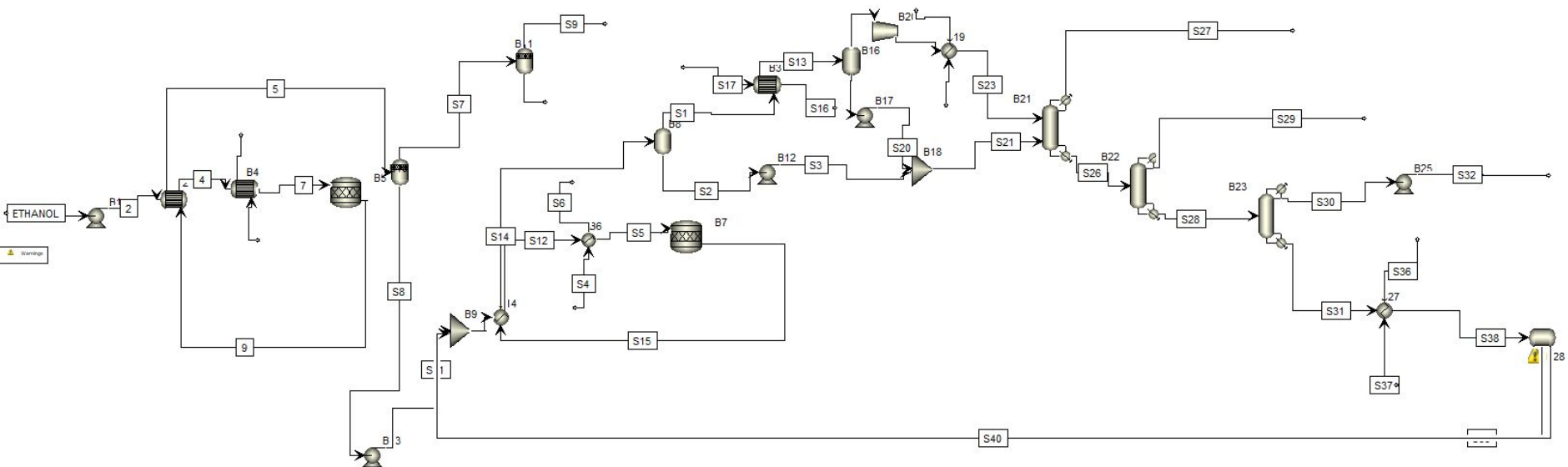
Sent to sheet 'Annual TPC'					
Utility	Default unit cost	Default cost units	Annual utility requirement, in appropriate units	Default units of utility requirement	Annual utility cost, million \$/y
Air, compressed					
Process air	0.45	\$/100m ³ #	2000000	100 m ³ /y	0.900
Instrument air	0.90	\$/100m ³ #	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											