

Acetaldehyde Production by Ethanol Dehydrogenation

Background

Acetaldehyde is a colorless liquid with a pungent, fruity odor. It is primarily used as a chemical intermediate, principally for the production of acetic acid, pyridine and pyridine bases, peracetic acid, pentaerythritol, butylene glycol, and chloral. Acetaldehyde is a volatile and flammable liquid that is miscible in water, alcohol, ether, benzene, gasoline, and other common organic solvents. The goal of this project is to design a grass-roots facility that is capable of producing 95,000 tons of acetaldehyde per year by ethanol dehydrogenation.

Process Description

A preliminary base case BFD for the overall process is shown in Figure 1.

Unit 100

A PFD of Unit 100 is shown in Figure 2. Ethanol, an 85-wt.% solution in water, Stream 1, is combined with 85-wt.% ethanol recycle stream, Stream 23, from Unit 200. The resultant stream, Stream 2, is then pumped to 100 psia and heated to 626°F in E-101 and E-102 before being fed to R-101, an isothermal, catalytic, packed-bed reactor, where the ethanol is dehydrogenated to form acetaldehyde. The reactor effluent is then cooled in E-103 and E-104. The resultant two-phase stream, Stream 8, is then separated in V-101. The vapor, Stream 9, is sent to T-101 where it is contacted with water, which absorbs the acetaldehyde and ethanol from the vapor stream. The resulting vapor effluent, Stream 11, is then sent for further processing and recovery of valuable

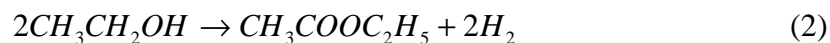
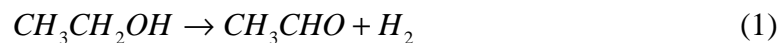
hydrogen. Alternatively, this stream could be used as fuel. Stream 12, the liquid, is combined with Stream 14, the liquid effluent from V-101, and sent to Unit 200.

Unit 200

A PFD for Unit 200 is shown in Figure 3. Stream 15 enters T-201 where the crude acetaldehyde, Stream 16, exits as the distillate. This crude acetaldehyde is then sent to T-203 where the acetaldehyde is purified to 99.9-wt.%, Stream 17. The bottoms, Stream 18, is sent to waste treatment. The bottoms from T-201, Stream 19, is sent to T-202 to begin the purification process of ethanol. In T-202, ethyl acetate and some water is removed from Stream 19 and exits as the distillate, Stream 20, which is then sent to waste treatment. The bottoms, Stream 21, is sent to T-204 where ethanol is separated from butanol, ethyl acetate, and most of the water. These impurities exit in Stream 22 and are sent to waste treatment. The distillate consists of an 85-wt.% solution of ethanol, which is then recycled back to Unit 100 to be used in the feed. Waste streams, Streams 18, 20, and 22, all contain small quantities of valuable chemicals. Methods for their separation and purification should be investigated.

Necessary Information and Simulation Hints

The following reactions occur during the dehydrogenation of ethanol:



The conversion of ethanol is assumed to be 60.8%. The yields for each reaction are as follows:

- (1) acetaldehyde 91.7%
- (2) ethyl acetate 3.8%
- (3) butanol 2.4%
- (4) acetic acid 2.1%

References are not available for these values. Since reaction kinetics were not available, the above conversions were assumed in the design of the process.

NRTL thermodynamics was used for K -values, as suggested by the Chemcad expert system.

Equipment Summary

E-101	Reactor Preheater
E-102	Reactor Preheater
E-103	Heat Exchanger
E-104	Heat Exchanger
E-105	Heat Exchanger
E-201	Condenser
E-202	Reboiler
E-203	Condenser
E-204	Reboiler
E-205	Condenser
E-206	Reboiler
E-207	Condenser
E-208	Reboiler
H-101	Fired Heater

P-101A/B	Feed Pump
P-102A/B	Dowtherm A Pump
P-201A/B	Reflux Pump
P-202A/B	Reflux Pump
P-203A/B	Reflux Pump
P-204A/B	Reflux Pump
T-101	Absorber
T-201	Distillation Column
T-202	Distillation Column
T-203	Distillation Column
T-204	Distillation Column
V-101	Flash Vessel
V-201	Reflux Vessel
V-202	Reflux Vessel
V-203	Reflux Vessel
V-204	Reflux Vessel

Stream Tables

Stream	1	2	3	4	5	6
Temp. (°F)	107.6	166.0	166.6	382.8	626.0	626.0
Press. (psia)	14.7	14.7	100	96.2	96.2	96.2
Vapor Fraction	0.0	0.0	0.0	1.0	1.0	1.0
Total Flow (lbmol/h)	1037.9	1498.7	1498.7	1498.7	1498.7	2076.0
Component Flows (lbmol/h)						
Acetaldehyde	--	2.4	2.4	2.4	2.4	546.6
Acetic Acid	--	--	--	--	--	11.8
Butanol	--	2.3	2.3	2.3	2.3	15.8
Water	336.8	464.6	464.6	464.6	464.6	466.3
Ethanol	701.1	1028.9	1028.9	1028.9	1028.9	403.3
Ethyl Acetate	--	0.4	0.4	0.4	0.4	21.7
Hydrogen	--	--	--	--	--	610.4

Stream	7	8	9	10	11	12
Temp. (°F)	387.9	157.0	107.3	152.3	152.6	152.2
Press. (psia)	96.1	95.1	94.3	94.3	94.3	94.3
Vapor Fraction	1.0	0.4	1.0	0.0	1.0	0.0
Total Flow (lbmol/h)	2076.0	2076.0	683.6	3600.1	638.1	3645.7
Component Flows (lbmol/h)						
Acetaldehyde	546.6	546.6	63.4	--	0.9	62.5
Acetic Acid	11.8	11.8	--	--	--	--
Butanol	15.8	15.8	--	--	--	--
Water	466.3	466.3	5.7	3600.1	26.9	3578.9
Ethanol	403.3	403.3	3.2	--	--	3.2
Ethyl Acetate	21.7	21.7	0.9	--	0.2	0.7
Hydrogen	610.4	610.4	610.4	--	610.4	0.2

Stream	13	14	15	16	17	18
Temp. (°F)	107.3	209.0	173.8	190.1	184.5	259.9
Press. (psia)	94.3	94.3	94.3	94.3	94.3	94.3
Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow (lbmol/h)	1392.4	1392.4	5037.7	603.5	539.0	64.6
Component Flows (lbmol/h)						
Acetaldehyde	483.2	483.2	545.7	543.2	537.7	5.4
Acetic Acid	11.7	11.7	11.8	--	--	--
Butanol	15.8	15.8	15.8	0.1	--	0.1
Water	460.6	460.6	4039.5	55.6	1.2	54.4
Ethanol	400.1	400.1	403.3	2.5	--	2.4
Ethyl Acetate	20.8	20.8	21.5	2.2	--	2.1
Hydrogen	--	--	--	--	--	--

Stream	19	20	21	22	23
Temp. (°F)	293.4	267.2	297.4	315.1	274.9
Press. (psia)	94.3	94.3	94.3	94.3	94.3
Vapor Fraction	0.0	0.0	0.0	0.0	0.0
Total Flow (lbmol/h)	4435.1	54.3	4380.7	3920.0	460.7
Component Flows (lbmol/h)					
Acetaldehyde	2.4	--	2.4	--	2.4
Acetic Acid	11.7	--	11.7	11.7	--
Butanol	15.8	--	15.8	13.4	2.4
Water	3985.0	11.3	3973.7	3845.8	127.9
Ethanol	400.9	24.1	376.8	49.0	327.8
Ethyl Acetate	19.4	19.0	0.4	--	0.4
Hydrogen	--	--	--	--	--

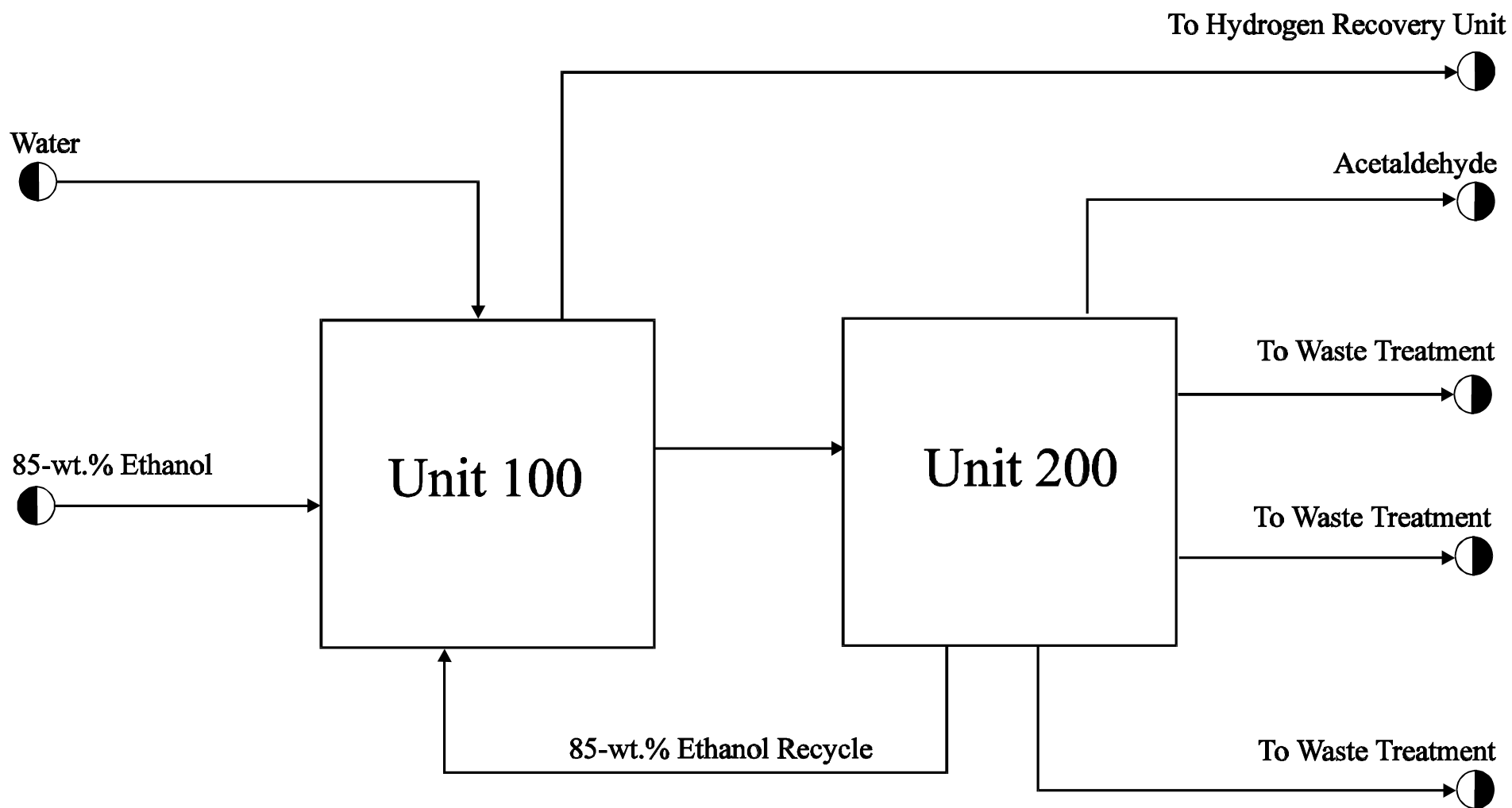


Figure 1: BFD for Overall Process

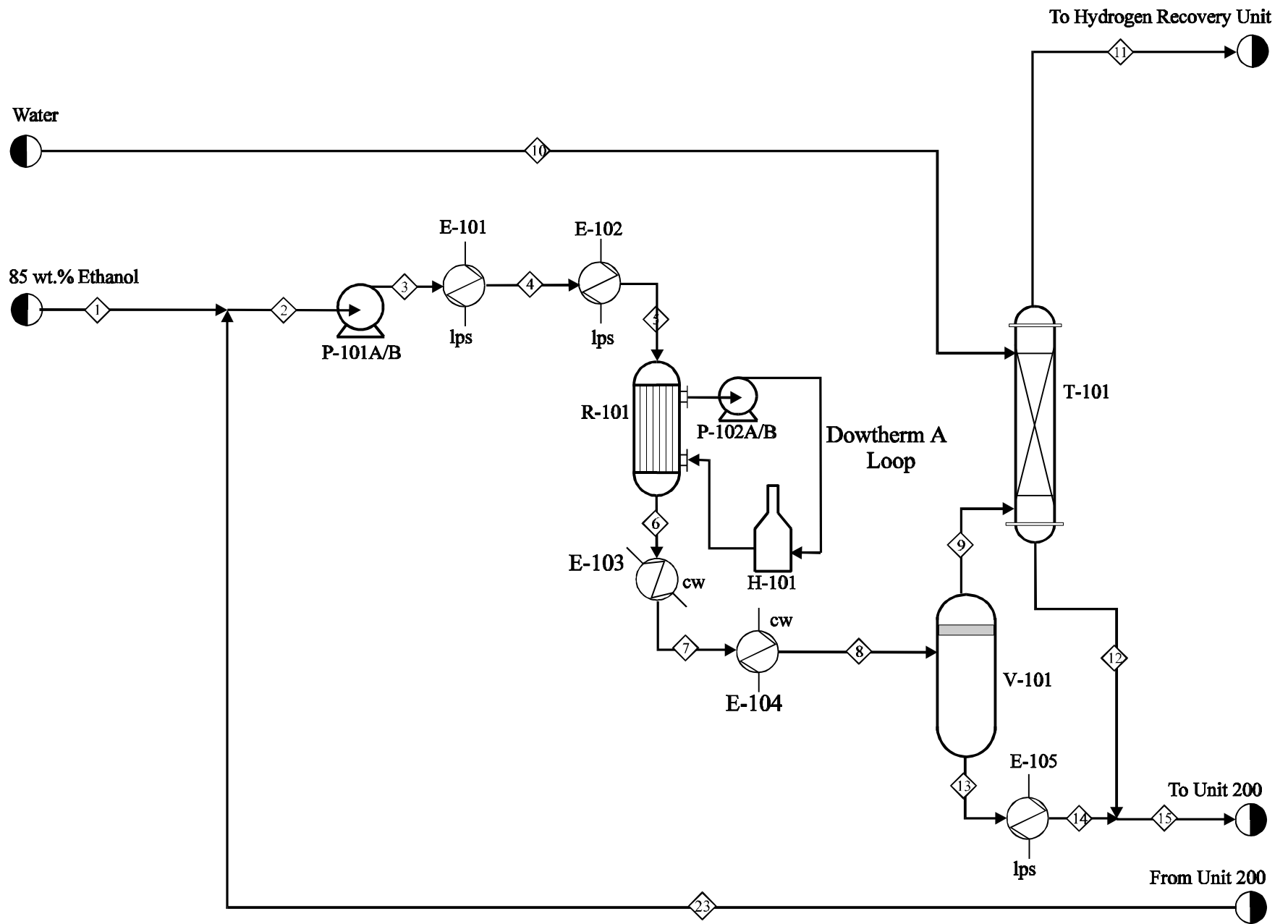


Figure 2: PFD for Unit 100

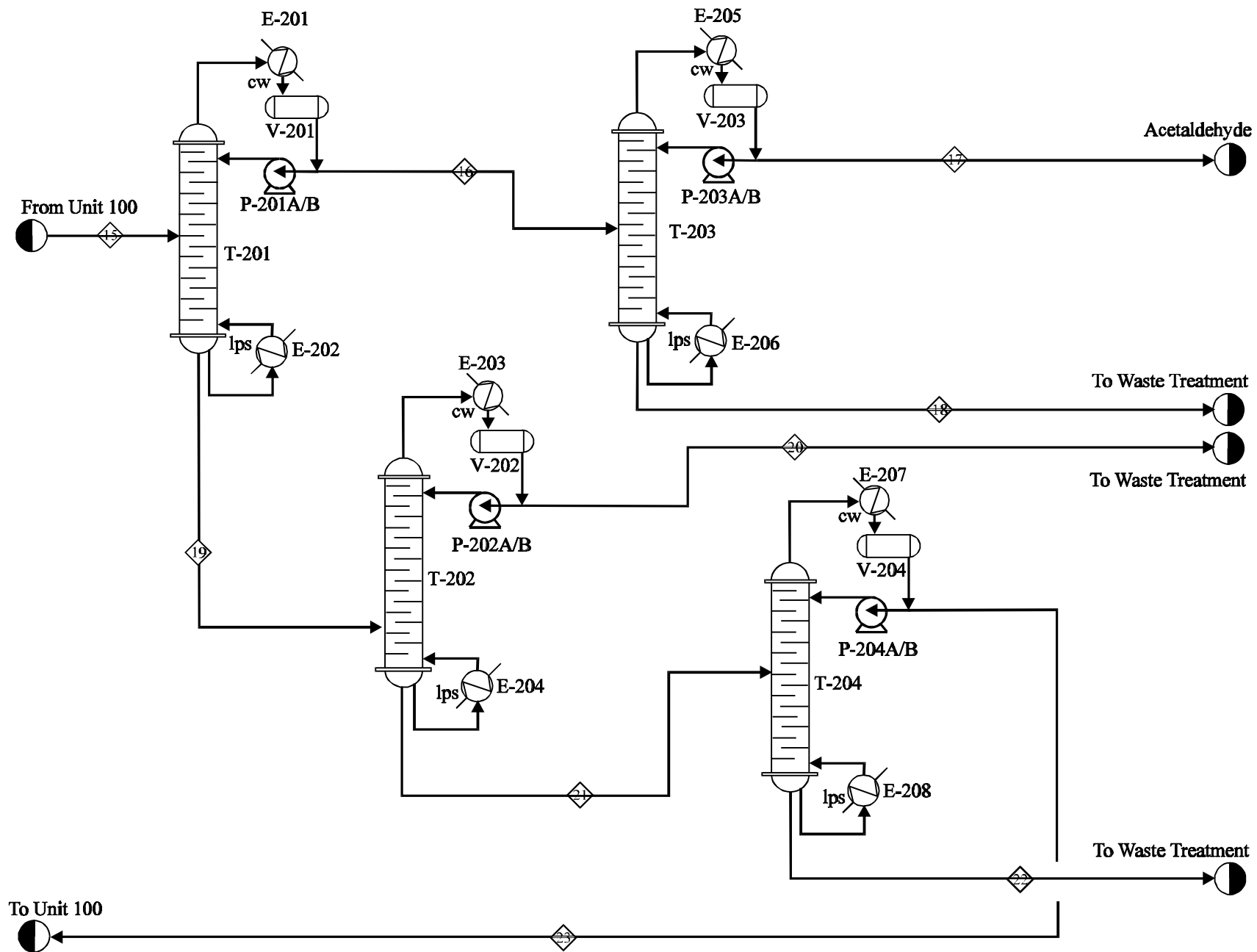


Figure 3: PFD for Unit 200