FINAL REPORT for the 2002 NSF-REU Site at
UIC, Department of Chemical Engineering

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Pollution Prevention in Pharmaceutical Batch Manufacturing

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Abstract

We, the laboratory for product and process design, are currently working on a waste treatment selection program for a pharmaceutical plant's process and the byproducts it generates. In order to understand material and energy flows, I modeled a chemical recipe for the manufacturing of a drug. Through mapping a hypothetical model, I was better equipped with the knowledge of how the waste streams are generated from the production of a desired product. This software package helped me understand the series of operations, such as reactions in a batch reactor, concentration and extraction on liquids, centrifuging, washing, and drying solids, and basic charging and transferring of material from vessel to vessel. Each stage converts raw materials into a stage intermediate through a series of twenty to sixty operations.

In addition to the case study, a refined model of the current incinerator model was produced—one in which gives a more detailed analysis of the sulfur and certain heavy metal combustion chemistry. Before I embarked on this project, the incineration model consisted of a hydrogen, carbon, oxygen, and nitrogen pathway through high temperature combustion. Heavy metals in general, plus inorganic solids, acids, and bases, and inert gases and water were all sent to a residue stream.

Introduction

The Environmental Protection Agency (EPA) has a set of guidelines and limitations it puts on industry in order to keep pollution at a minimum. Pollution prevention consists of all those activities that reduce the generation of hazardous waste. There are several terms which describe this activity, such as waste minimization, waste reduction, source reduction, waste diversion, pollution prevention, recycling, and reuse. The term "hazardous waste" means a solid waste or combination of solid wastes which because of its quantity, concentration, or physical, chemical or infectious characteristics, may cause or significantly contribute to an increase in mortality or an increase in serious, irreversible, or incapacitating reversible illness, or pose a substantial present or potential hazard to human health or the environment when improperly treated, stored, transported, disposed of, or otherwise managed.

In a recent policy statement, the EPA suggested the following hierarchy for management of

wastes: (i) source reduction, (ii) recycling, and (iii) treatment disposal. Source reduction would include perhaps lowering the quantity of potential pollutants that already are present in raw feed material. Some byproducts, however, may be of value, or even an important resource, and therefore the option of recycling should be implemented on-site if possible, or off-site otherwise if found to still be profitable. The last resort would be to dispose of the waste, if it is under allowable concentration, by atmosphere (gas emissions), sewer (liquid waste), or landfill (solid residue).

The waste streams that are produced must be introduced into some kind of treatment option in order to destroy all toxic substances. There are five main categories within our waste treatment plan: (i) physical separation, (ii) chemical separation, (iii) biological treatment, (iv) thermal treatment, and (v) final treatment.

Outline: In this report, Part 1 will discuss the overview of the case study followed by a detailed description of each of the six stages. Part 2 will discuss the automated treatment selector and give an application of the first stage's waste streams. Part 3 will go more into detail about the reaction mechanism which was refined in our incinerator model, and finally the fourth section will give the conclusions.

1. Manufacturing of a Maleate Salt (Merck Case Study):

Our case study consists of a batch of six stages of a pharmaceutical process producing a maleate salt. The outcome is shown in Figure 1.7 in Section 2.2. Appendix A shows all the streams of each stage organized in table format.

The objective of this case study is to map a "cradle to grave" batch process and analyze how the waste streams are produced and from which operations they spawn. The following sections discuss in more detail each of the stages' main operations in addition to the waste streams in the case study.

1.1. Detailed Discussion of Individual Process Stages:

In this section each of the individual stages will be discussed in detail. In stages one through six, the main operations are GRIGNARD reaction in stage one, then two extractions using THF

as solvent. In the second stage, the DISSOLUTION, HYDROXYAMINATION, NEUTRALIAZATION-2, and NEUTRALIZATION-1 reactions are carried out in that respective order, and then two extractions using sodium chloride, acetonitrile, and methylene chloride as solvents. Stage 3 contains basically just the RING-CLOSURE reaction. In Stage 4, the HYDROGENOLYSIS reaction is the only reaction, but there are four extraction operations. The first uses toluene as solvent, the second and third both use isopropyl acetate as solvent utilizing the same extraction data, and the fourth also contains isopropyl acetate as solvent. The fifth stage first performs two extractions using methylene chloride as solvent, and then the SALT-FORMATION reaction is introduced. For the final production stage,

For many of the stages, certain operations were given warning messages and suggestions as to how to improve the stage in order to overcome realistic problems that may come about from the subsequent steps. The older version of this program was written with much less constriction set upon the series of steps involved in each stage, but the newer version with which I modeled the original case study with was not as "forgiving."

1.2. Stage 1—GRIGNARD Process Summary:

The main raw material here is trienone ($C_{15}H_{10}O$), and the main intermediate product is carbinol ($C_{16}H_{14}O$). The main operations throughout this case are: an isothermal reaction in tank ST-100 via GRIGNARD, followed by two extraction steps, an evacuation, four concentrations, a centrifuge, and finally a drying. The GRIGNARD reaction is:

1 TRIENONE + 1 MEMGBR + 2 ACETIC ACID -> 1 CARBINOL + 0.5 MAGNESIUM BROMIDE +
0.5 MAGNESIUM HYDROXIDE + 1 ACETIC ANHYDRIDE

The batch cycle time is 21.87 hours, and the batch recipe in its entirety is shown in Table 1.2.1.

Table 1.Operating Steps for Stage 1 - GRIGNARD

Step 1. Start
Step 1.1. CHARGE 111 kg of WATER to ST-100, with condenser outlet temperature 20 ºC
Step 1.2. CHARGE 20 kg of SODIUM ACETATE to ST-100, with condenser outlet temperature 20 ºC
Step 1.3. CHARGE 14.60 kg of ACETIC ACID to ST-100, with condenser outlet temperature 20 ºC
Step 1.4. CHARGE 44.40 kg of TETRAHYDROFURAN to ST-101, with condenser outlet temperature 20 ºC
Note: THF is sieve dried.
Step 1.5. CHARGE 24.25 kg of TRIENONE to ST-101, with condenser outlet temperature 20 ºC
Step 1.6. CHARGE 55.50 kg of TETRAHYDROFURAN to ST-102, with condenser outlet temperature 20 ºC
Note: THF is sieve dried.
Note: Check for kf.

Step 1.7. CHARGE 61.30 kg of MEMGBR-ETHER-3M to ST-102, with condenser outlet temperature 20 ºC

Step 1.8. TRANSFER 100 wt% of the content of ST-101 to ST-102 , with condenser outlet temperature 20 ºC

Step 1.9. AGE ST-102, for 60 min, and maintain temperature

Step 1.10. COOL ST-102 to 12.50 ºC

Step 1.11. COOL ST-100 to 10 ºC

Step 1.12. REACT in ST-100 isothermally, for 120 min, while adding 100 wt% of the content in ST-102, via [GRIGNARD, Rank: 1, conversion: 99.00%, yield: 97.00%]

Step 1.13. CHARGE 44.40 kg of TETRAHYDROFURAN to ST-102, with condenser outlet temperature 20 ºC

Step 1.14. TRANSFER 100 wt% of the content of ST-102 to ST-100 , with condenser outlet temperature 20 ºC

Step 1.15. TRANSFER 100 wt% of the content of ST-100 to EX-100 , with condenser outlet temperature 20 ºC

Step 1.16. EXTRACT in EX-100, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-31}, sending bottom layer to TA-100, giving the name Bottom-Layer with condenser outlet temperature 20 ºC

Step 1.17. TRANSFER 100 wt% of the content of TA-100 to Disposal-100 , the transferred portion being named 1st-AQ-Waste-Layer, with condenser outlet temperature 20 ºC

Step 1.18. CHARGE 62.50 kg of SODIUM CHLORIDE to EX-100, with condenser outlet temperature 20 ºC

Step 1.19. EXTRACT in EX-100, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-31}, sending bottom layer to TA-101, giving the name Bottom-Layer with condenser outlet temperature 20 ºC

Step 1.20. TRANSFER 100 wt% of the content of TA-101 to Disposal-101 , the transferred portion being named 2nd-AQ-Waste-Layer, with condenser outlet temperature 20 ºC

Step 1.21. TRANSFER 100 wt% of the content of EX-100 to ST-103 , with condenser outlet temperature 20 ºC

Step 1.22. EVACUATE ST-103 to 18 kPa, operating 15 min, with condenser outlet temperature 20 ºC, send non condensed gas to Atm_1

Step 1.23. CONCENTRATE batch in ST-103, using model Rayleigh distill with parameter(s): {distillate volume reaches 60.01 l,using TETRAHYDROFURAN as key compound}, naming the distillate as Distillate and sending distillate to receiver VR-100, through condenser CN-100 with outlet temperature 20 ºC, using utility Low Temperature Glycol

Step 1.24. TRANSFER 100 wt% of the content of VR-100 to SolvRec-100 , the transferred portion being named THF-DIST, with condenser outlet temperature 20 ºC

Step 1.25. CHARGE 227.3 l of CYCLOHEXANE to ST-103, with condenser outlet temperature 20 ºC

Note: Carbinol crystallizes.

Step 1.26. CONCENTRATE batch in ST-103, using model Rayleigh distill with parameter(s): {distillate volume reaches 60.01 l,using TETRAHYDROFURAN as key compound}, naming the distillate as Distillate and sending distillate to receiver VR-101, through condenser CN-100 with outlet temperature 20 ºC

Step 1.27. TRANSFER 100 wt% of the content of VR-101 to TA-102 , with condenser outlet temperature 20 ºC

Step 1.28. CHARGE 227.3 l of CYCLOHEXANE to ST-103, with condenser outlet temperature 20 ºC

Step 1.29. CONCENTRATE batch in ST-103, using model Rayleigh distill with parameter(s): {distillate volume reaches 60.01 l,using TETRAHYDROFURAN as key compound}, naming the distillate as Distillate and sending distillate to receiver VR-102, through condenser CN-100

Step 1.30. TRANSFER 100 wt% of the content of VR-102 to TA-102 , with condenser outlet temperature 20 ºC

Step 1.31. TRANSFER 100 wt% of the content of TA-102 to SolvRec-101 , the transferred portion being named 1st-CYHX-DIST, with condenser outlet temperature 20 ºC

Step 1.32. CHARGE 227.3 l of CYCLOHEXANE to ST-103, with condenser outlet temperature 20 ºC

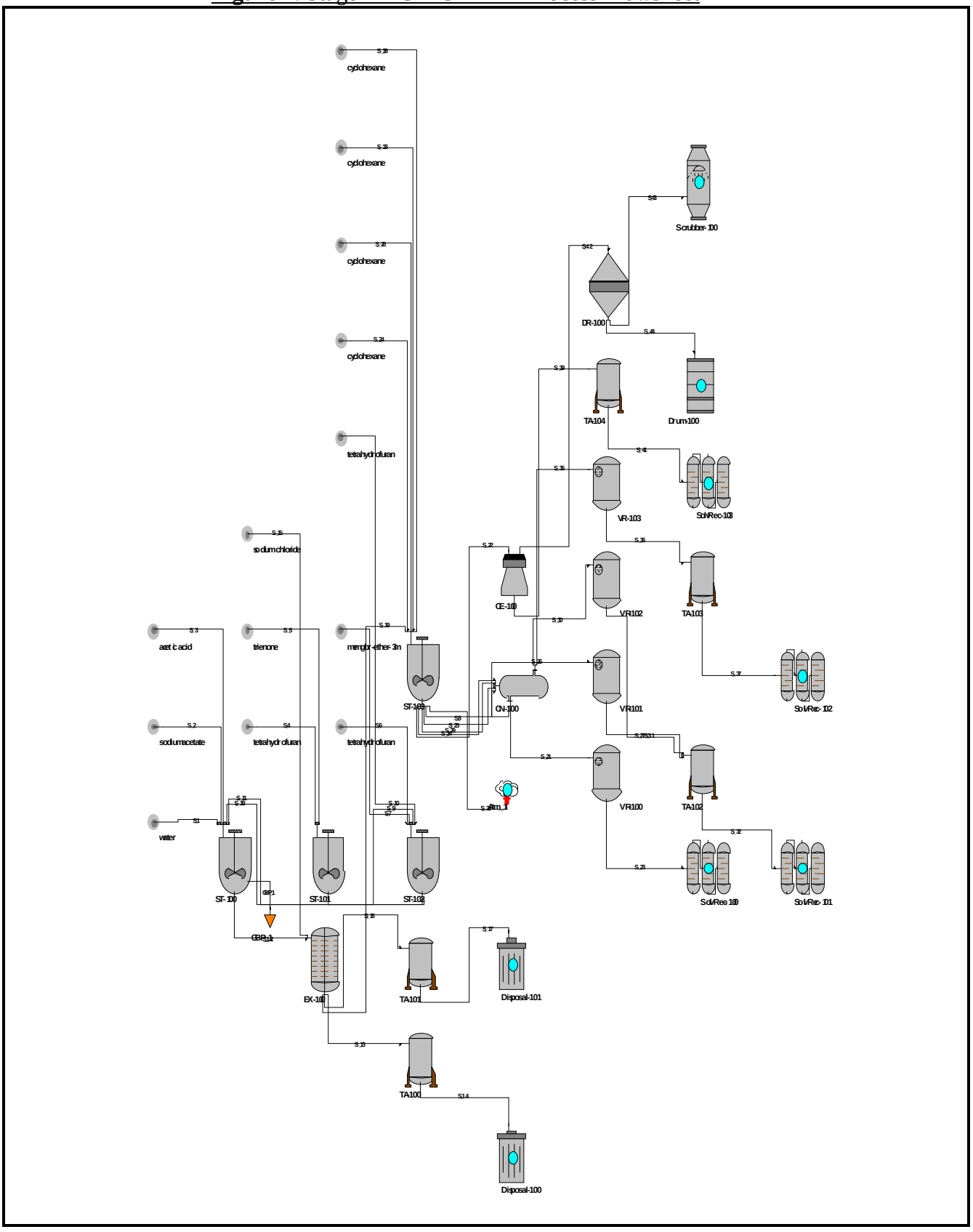
Step 1.33.	CONCENTRATE batch in ST-103, using model Rayleigh distill with parameter(s): {distillate volume reaches 60.01 l,using TETRAHYDROFURAN as key compound}, naming the distillate as Distillate and sending distillate to receiver VR-103, through condenser CN-100 with outlet temperature 20 ºC
Step 1.34.	TRANSFER 100 wt% of the content of VR-103 to TA-103 , with condenser outlet temperature 20 ºC
Step 1.35.	TRANSFER 100 wt% of the content of TA-103 to SolvRec-102 , the transferred portion being named 2nd-CYHX-DIST, with condenser outlet temperature 20 ºC
Step 1.36.	CHARGE 313.7 l of CYCLOHEXANE to ST-103, with condenser outlet temperature 20 ºC
Step 1.37.	COOL ST-103 to 10 ºC
Step 1.38.	AGE ST-103, for 120 min, and maintain temperature
Step 1.39.	CENTRIFUGE 100 wt% of batch from ST-103 in CE-100 for 1 time(s), separating materials [97.0000 wt%, CARBINOL] as solid, lod of cake 10 wt% liquid in total mass, sending mother-liquor to TA-104, cake stays in CE-100, total operation time 240 min, with condenser outlet temperature 20 ºC
Step 1.40.	TRANSFER 100 wt% of the content of TA-104 to SolvRec-103 , the transferred portion being named CYHX-ML, with condenser outlet temperature 20 ºC
Step 1.41.	TRANSFER 100 wt% of the content of CE-100 to DR-100 , with condenser outlet temperature 20 ºC
Step 1.42.	DRY in DR-100, at 25 ºC, for 480 min, sending vapor to Scrubber-100 , with loss on drying 0.10000 wt% liquid in total mass
Step 1.43.	TRANSFER 100 wt% of the content of DR-100 to Drum-100 , the transferred portion being named CARBINOL-CRUDE

Also, the BDK software allows the user to run a process summary report for each stage, and Table 1.2 shows a waste stream table of all the effluent streams included within this stage. Stream 14 is the first aqueous waste layer, S_17 is the second aqueous waste layer, S_23 is a tetrahydrofuran (THF) distillate, S_32 is the first cyclohexane distillate, S_37 is the second cyclohexane distillate, S_41 is the cyclohexane mother liquor that forms during the centrifuge operation, and S_44 is crude carbinol. Figure 1.1 is a thorough flowsheet of the complete process.

Table 2. Waste Stream Table of Stage 1 – GRIGNARD

	S_14	S_17	S_23	S_32	S_37	S_41	S_44
ORIGIN	TA-100	TA-101	VR-100	TA-102	TA-103	TA-104	DR-100
DESTINATION	Disposal-100	Disposal-101	CE-100	SolvRec-101	SolvRec-102	SolvRec-103	Drum-100
TOTAL MASS (kg)	204.340	68.650	734.288	97.262	47.540	707.766	23.890
VOLUME (m^3)	0.165	0.035	0.909	0.120	0.060	0.892	0.013
DENSITY	1235.982	1943.117	807.708	810.388	792.213	793.023	1797.645
TEMPERATURE (C)	10.984	20.000	10.000	20.000	20.000	10.000	25.000
PRESSURE (kPa)	101.325	101.325	18.000	101.325	101.325	101.325	101.325
PHASE	Liquid	Solid	Liquid	Liquid	Liquid	Liquid	Solid
COMPOSITION (kg per kg of batch)							
Water	107.767	3.139	0.081	0.007	0.002	0.078	0.000
sodium acetate	20.001	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.619	0.000	0.000	0.000	0.000	0.000	0.000
Tatrahydrofuran	2.830	2.774	45.107	32.361	7.283	44.943	0.001
Trienone	0.243	0.000	0.000	0.000	0.000	0.000	0.000
ether-3M	29.505	0.000	0.000	0.000	0.000	0.000	0.000
MEMGBR	17.917	0.000	0.000	0.000	0.000	0.000	0.000
Carbinol	0.249	0.246	24.606	0.000	0.000	0.736	23.866
magnesium bromide	10.395	0.000	0.000	0.000	0.000	0.000	0.000
magnesium hydroxide	3.292	0.000	0.000	0.000	0.000	0.000	0.000
acetic anhydride	11.527	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	62.500	0.000	0.000	0.000	0.000	0.000
Cyclohexane	0.000	0.000	664.494	64.894	40.263	662.009	0.022

Figure 1. Stage 1 – GRIGNARD Process Flowsheet



1.3. Stage 2—HYDROXYAMINATION Process Summary:

In this case, the carbinol from the previous case is the main raw material and hydroxamine ($C_{16}H_{15}NO$) is the intermediate product. Throughout the case, parallel and sequential operations run simultaneously. First, the DISSOLUTION reaction takes place, then HYDROXYAMINATION, followed by NEUTRALIZATION-2 (isothermally) and then NEUTRALIZATION-1. Two extractions, an evacuation, two concentrations, a centrifuge, and a washing and drying end Case 2. The four reactions proceed as follows:

DISSOLUTION: 1 SODIUM ACETATE + 1 HYDROXYLAMINE-HYDROCHLORIDE -> 1 SODIUM CHLORIDE + 1 ACETIC ACID + 1 HYDROXYLAMINE

HYDROXYAMINATION: 1 CARBINOL + 1 HYDROXYLAMINE -> 1 WATER + 1 HYDROXAMINE

NEUTRALIZATION-2: 1 DICHLOROACETIC ACID + 1 AMMONIUM HYDROXIDE -> 1 WATER + 1 AMMONIUM-DICHLOROACETATE-CASE2

NEUTRALIZATION-1: 1 AMMONIUM HYDROXIDE + 1 ACETIC ACID -> 1 AMMONIUM ACETATE + 1 WATER

The batch cycle time is 271.4 hours, and the batch recipe is shown in Table 1.3.

Table 3. Operating Steps for Stage 2 – HYDROXYAMINATION

Step 1.	Start
Step 1.1.	PARALLEL START
Step 1.2.	SEQUENTIAL START
Note:	acetone-nitrile is sieve dried
Step 1.3.	CHARGE 44.40 kg of ACETONE-NITRILE to ST-100, with condenser outlet temperature 20 ºC
Note:	Methylene-chloride is sieve dried
Step 1.4.	CHARGE 187.8 kg of METHYLENE CHLORIDE to ST-100, with condenser outlet temperature 20 ºC
Step 1.5.	CHARGE 29.50 kg of HYDROXYLAMINE-HYDROCHLORIDE to ST-100, with condenser outlet temperature 20 ºC
Note:	Sodium acetate must be anhydrous
Step 1.6.	CHARGE 34.70 kg of SODIUM ACETATE to ST-100, with condenser outlet temperature 20 ºC
Step 1.7.	CHARGE 55.20 kg of DICHLOROACETIC ACID to ST-100, with condenser outlet temperature 20 ºC
Step 1.8.	SEQUENTIAL END
Step 1.9.	SEQUENTIAL START
Step 1.10.	CHARGE 125.1 kg of METHYLENE CHLORIDE to TA-100, with condenser outlet temperature 20 ºC
Step 1.11.	CHARGE 7.400 kg of ACETONE-NITRILE to TA-100, with condenser outlet temperature 20 ºC
Step 1.12.	CHARGE 23.60 kg of CARBINOL to TA-100, from Drum-100, with condenser outlet temperature 20 ºC
Step 1.13.	SEQUENTIAL END

Step 1.14.	PARALLEL END
Step 1.15.	HEAT ST-100 to 47 ºC , with condenser outlet temperature 20 ºC
Step 1.16.	AGE ST-100, for 30 min, and maintain temperature
Step 1.17.	REACT in ST-100 isothermally, for 120 min, while adding 100 wt% of the content in TA-100, via [DISSOLUTION, Rank: 1, conversion: 100.00%, yield: 100.00%], using Brine
Step 1.18.	REACT in ST-100 isothermally, for 120 min, via [HYDROXYAMINATION, Rank: 1, conversion: 99.00%, yield: 98.00%], using Brine
Step 1.19.	CHARGE 31.30 kg of METHYLENE CHLORIDE to TA-100, with condenser outlet temperature 20 ºC
Step 1.20.	TRANSFER 100 wt% of the content of TA-100 to ST-100 , with condenser outlet temperature 20 ºC
Step 1.21.	AGE ST-100, for 240 min, and maintain temperature
Step 1.22.	COOL ST-100 to 15 ºC, using Low Temperature Glycol
Step 1.23.	CHARGE 221.8 kg of 15%AMMONIUM-HYDROXIDE to TA-101, with condenser outlet temperature 20 ºC
Step 1.24.	REACT in ST-100 isothermally, for 120 min, while adding 100 wt% of the content in TA-101, via [NEUTRALIZATION-2, Rank: 1, conversion: 100.00%, yield: 100.00%], using Super Heated Steam
Step 1.25.	CHARGE 46 kg of ACETIC ACID to ST-100, with condenser outlet temperature 20 ºC
Step 1.26.	REACT in ST-100 isothermally, for 120 min, via [NEUTRALIZATION-1, Rank: 1, conversion: 100.00%, yield: 100.00%], using Brine
Step 1.27.	TRANSFER 100 wt% of the content of ST-100 to EX-100 , with condenser outlet temperature 20 ºC
Step 1.28.	EXTRACT in EX-100, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-32-3}, sending bottom layer to EX-101, giving the name Bottom-Layer with condenser outlet temperature 20 ºC
Step 1.29.	TRANSFER 100 wt% of the content of EX-100 to TA-102 , with condenser outlet temperature 20 ºC
Step 1.30.	TRANSFER 100 wt% of the content of TA-102 to Disposal-100 , the transferred portion being named AQ-NH4-SALT-LAYER, with condenser outlet temperature 20 ºC
Step 1.31.	CHARGE 141.3 kg of SODIUM CHLORIDE to EX-101, with condenser outlet temperature 20 ºC
Step 1.32.	EXTRACT in EX-101, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-32-3}, sending bottom layer to ST-101, giving the name Bottom-Layer with condenser outlet temperature 20 ºC
Step 1.33.	TRANSFER 100 wt% of the content of EX-101 to TA-103 , with condenser outlet temperature 20 ºC
Step 1.34.	TRANSFER 100 wt% of the content of TA-103 to Disposal-101 , the transferred portion being named AQ-NaCl-Layer, with condenser outlet temperature 20 ºC
Step 1.35.	EVACUATE ST-101 to 6.666 kPa, operating 15 min, with condenser outlet temperature 20 ºC, send non condensed gas to Atm_1
Step 1.36.	CONCENTRATE batch in ST-101, using model Rayleigh distill with parameter(s): {distillate volume reaches 35 l,using AMMONIUM ACETATE as key compound}, using heating utility Hot Water, naming the distillate as Distillate and sending distillate to receiver VR-100, through condenser CN-100 with outlet temperature 20 ºC
Step 1.37.	TRANSFER 100 wt% of the content of VR-100 to SolvRec-100 , the transferred portion being named MECl2-Dist, with condenser outlet temperature 20 ºC
Step 1.38.	CHARGE 92 kg of CYCLOHEXANE to ST-101, with condenser outlet temperature 20 ºC
Note:	Assuming ideal MeCl2-cyhx is incorrect
Step 1.39.	CONCENTRATE batch in ST-101, using model Rayleigh distill with parameter(s): {distillate volume reaches 120 l,using CYCLOHEXANE as key compound}, using heating utility Hot Water, naming the distillate as Distillate and sending distillate to receiver VR-101, through condenser CN-100 with outlet temperature 11 ºC

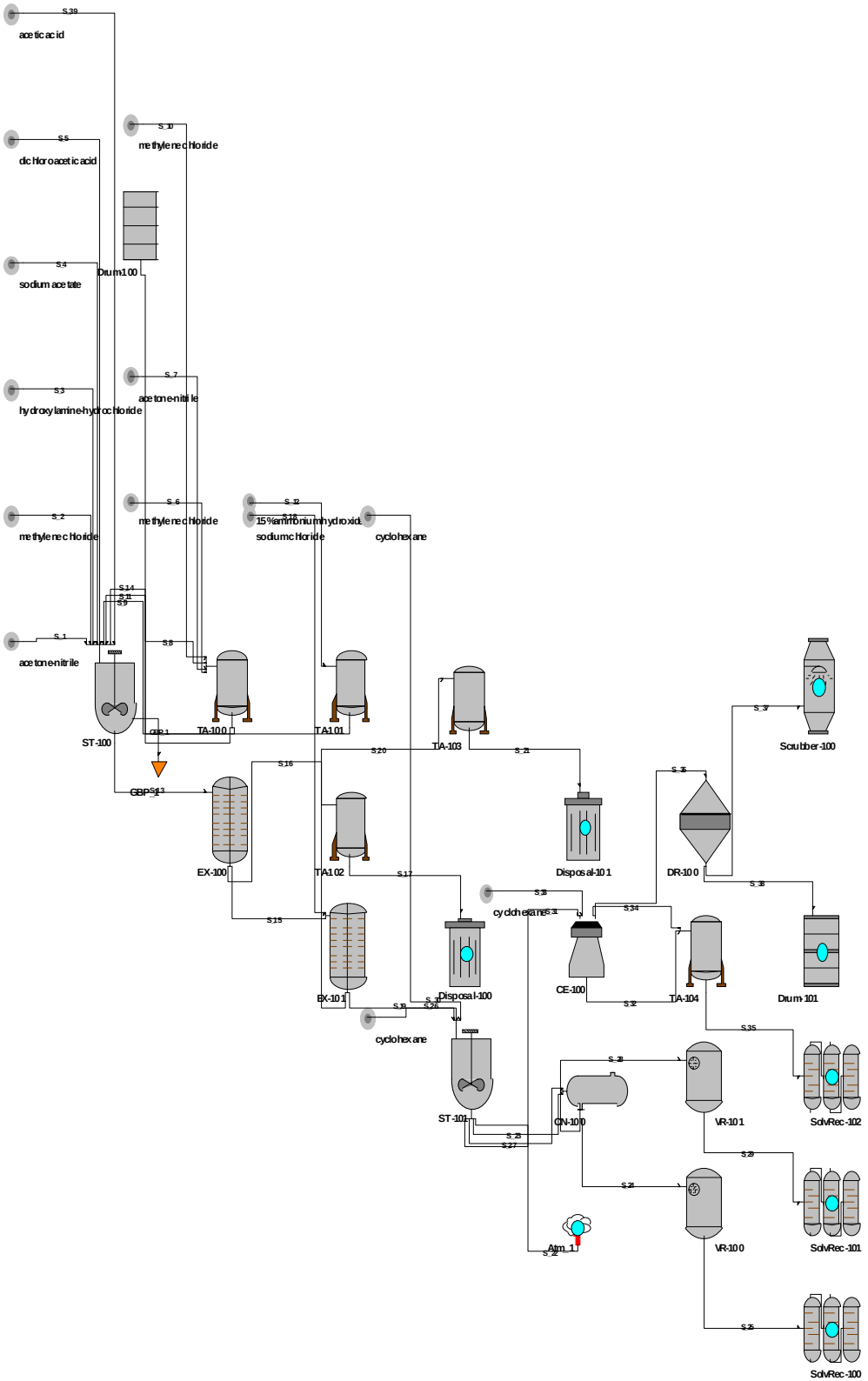
Step 1.40.	TRANSFER 100 wt% of the content of VR-101 to SolvRec-101 , the transferred portion being named MeCl2-Cyhx-Dist, with condenser outlet temperature 20 ºC
Note:	Hydroxamine crystallizes out
Step 1.41.	CHARGE 140.9 l of CYCLOHEXANE to ST-101, with condenser outlet temperature 20 ºC
Step 1.42.	COOL ST-101 to 9 ºC
Step 1.43.	AGE ST-101, for 120 min, and maintain temperature
Step 1.44.	CENTRIFUGE 100 wt% of batch from ST-101 in CE-100 for 1 time(s), separating materials [97.0000 wt%, HYDROXAMINE] as solid, lod of cake 10 wt% liquid in total mass, sending mother-liquor to TA-104, cake stays in CE-100, total operation time 240 min, with condenser outlet temperature 20 ºC
Step 1.45.	WASH CAKE in CE-100 with 140.9 l of CYCLOHEXANE, sending wash to TA-104, name it Spent-wash, assume displacement, lod of cake 20 wt% liquid in total mass, number of washes 1, operating time 14400 min per wash
Step 1.46.	TRANSFER 100 wt% of the content of TA-104 to SolvRec-102 , the transferred portion being named Cyhx-ML+Wash, with condenser outlet temperature 20 ºC
Step 1.47.	TRANSFER 100 wt% of the content of CE-100 to DR-100 , with condenser outlet temperature 20 ºC
Step 1.48.	DRY in DR-100, for 480 min, sending vapor to Scrubber-100 , with loss on drying 0.10000 wt% liquid in total mass
Step 1.49.	TRANSFER 100 wt% of the content of DR-100 to Drum-101 , the transferred portion being named Hydroxamine-crude

Table 1.4 shows a waste stream table of all the effluent streams included within this stage. Stream 17 is a liquid aqueous ammonium salt layer, S_21 is a solid aqueous sodium chloride layer, S_25 is a solid methylene chloride distillate, S_29 is a liquid methylene chloride cyclohexane distillate, S_35 is solid cyclohexane mother liquor wash, and S_38 is solid crude hydroxamine. Figure 1.2 is a thorough flowsheet of the complete process.

Table 4. Waste Stream Table of Stage 2 – HYDROXYAMINATION

	S_17	S_21	S_25	S_29	S_35	S_38
Origin	TA-102	TA-103	VR-100	VR-101	TA-104	DR-100
Destination	Disposal-100	Disposal-101	SolvRec-100	SolvRec-101	SolvRec-102	Drum-101
Total Mass (kg)	310.955	142.229	9.572	92.789	662.887	23.71
Volume (m^3)	0.285	0.067	0.035	0.12	0.521	0.013
Density (kg/m^3)	1090.65	2130.227	273.5	773.231	1272.103	1797.615
Temperature (C)	15.841	19.547	20	11	13.371	24.352
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Solid	Solid	Liquid	Solid	Solid
Composition (kg per kg batch)						
acetone-nitrile	0.000	0.000	0.000	0.000	51.798	0.000
Methylene chloride	0.345	0.344	0.000	0.000	343.515	0.000
hydroxylamine-hydrochloride	0.000	0.000	0.000	0.000	0.106	0.000
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000
dichloroacetic acid	0.000	0.000	0.000	0.000	0.000	0.000
Carbinol	0.000	0.001	0.000	0.000	0.232	0.000
Ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000
Water	195.336	0.778	0.000	0.000	0.000	0.000
acetic acid	0.000	0.000	0.002	0.000	0.000	0.000
sodium chloride	24.475	140.144	0.000	0.000	1.399	0.000
hydroxylamine	0.053	0.053	9.561	0.789	0.046	0.000
hydroxamine	0.012	0.013	0.000	0.000	0.736	23.686
Ammonium-dichloroacetate	0.000	0.000	0.000	0.000	53.071	0.000
Ammonium acetate	90.734	0.899	0.009	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	92.000	211.985	0.024

Figure 2. Stage 2 – HYDROXYAMINATION Process Flowsheet



1.4. Stage 3—N-HYDROXY Process Summary:

In this relatively short casestudy, hydroxamine is used to generate N-Hydroxy ($C_{16}H_{14}NO$), through the RING-CLOSURE reaction followed by filtration, washing, evacuation, concentration, and then another evacuation and concentration. The RING-CLOSURE reaction is:

1 HYDROXAMINE-IV + 1 ACETIC ACID + 1 POTASSIUM-BUTOXIDE -> 1 N-HYDROXY + 1 TERT-BUTYL-ALCOHOL + 1 KOAC

The batch cycle time is 98.26 hours, and the batch recipe is shown in Table 1.5.

Table 5. Operating Steps for Stage 3 – N-HYDROXY

Step 1.	Start
Step 1.1.	PARALLEL START
Step 1.2.	CHARGE 120.5 kg of ACETIC ACID to ST-100, with condenser outlet temperature 20 ºC
Step 1.3.	SEQUENTIAL START
Note:	THF must be sieve dried
Step 1.4.	CHARGE 204 kg of TETRAHYDROFURAN to ST-101, with condenser outlet temperature 20 ºC
Step 1.5.	CHARGE 13 kg of POTASSIUM-BUTOXIDE to ST-101, with condenser outlet temperature 20 ºC
Step 1.6.	CHARGE 23 kg of HYDROXAMINE-IV to ST-101, from Drum-101, with condenser outlet temperature 20 ºC
Step 1.7.	AGE ST-101, for 30 min, and maintain temperature
Step 1.8.	SEQUENTIAL END
Step 1.9.	PARALLEL END
Step 1.10.	REACT in ST-100 isothermally, for 120 min, while adding 100 wt% of the content in ST-101, via [RING-CLOSURE, Rank: 1, conversion: 99.00%, yield: 100.00%]
Step 1.11.	CHARGE 37 kg of TETRAHYDROFURAN to ST-101, with condenser outlet temperature 20 ºC
Step 1.12.	CHARGE 37 kg of ACETIC ACID to ST-101, with condenser outlet temperature 20 ºC
Step 1.13.	TRANSFER 100 wt% of the content of ST-101 to ST-100 , with condenser outlet temperature 20 ºC
Step 1.14.	AGE ST-100, for 30 min, and maintain temperature
Step 1.15.	FILTER 100 wt% of batch from ST-100 in FI-100, separating materials [100.0000 wt%, KOAC][100.0000 wt%, POTASSIUM-BUTOXIDE], as solid, lod of cake 30 wt% liquid in total mass, sending mother liquor to ST-102 , giving the name Mother-Liquor, operating time 240 min, with condenser outlet temperature 20 ºC
Step 1.16.	WASH CAKE in FI-100 with 45.46 l of TETRAHYDROFURAN, sending wash to ST-102, name it Spent-wash, assume displacement, lod of cake 20 wt% liquid in total mass, number of washes 1, operating time 5400 min per wash
Step 1.17.	PARALLEL START
Step 1.18.	TRANSFER 100 wt% of the content of FI-100 to Disposal-100 , the transferred portion being named THF-Wet-Cake, with condenser outlet temperature 20 ºC
Step 1.19.	SEQUENTIAL START

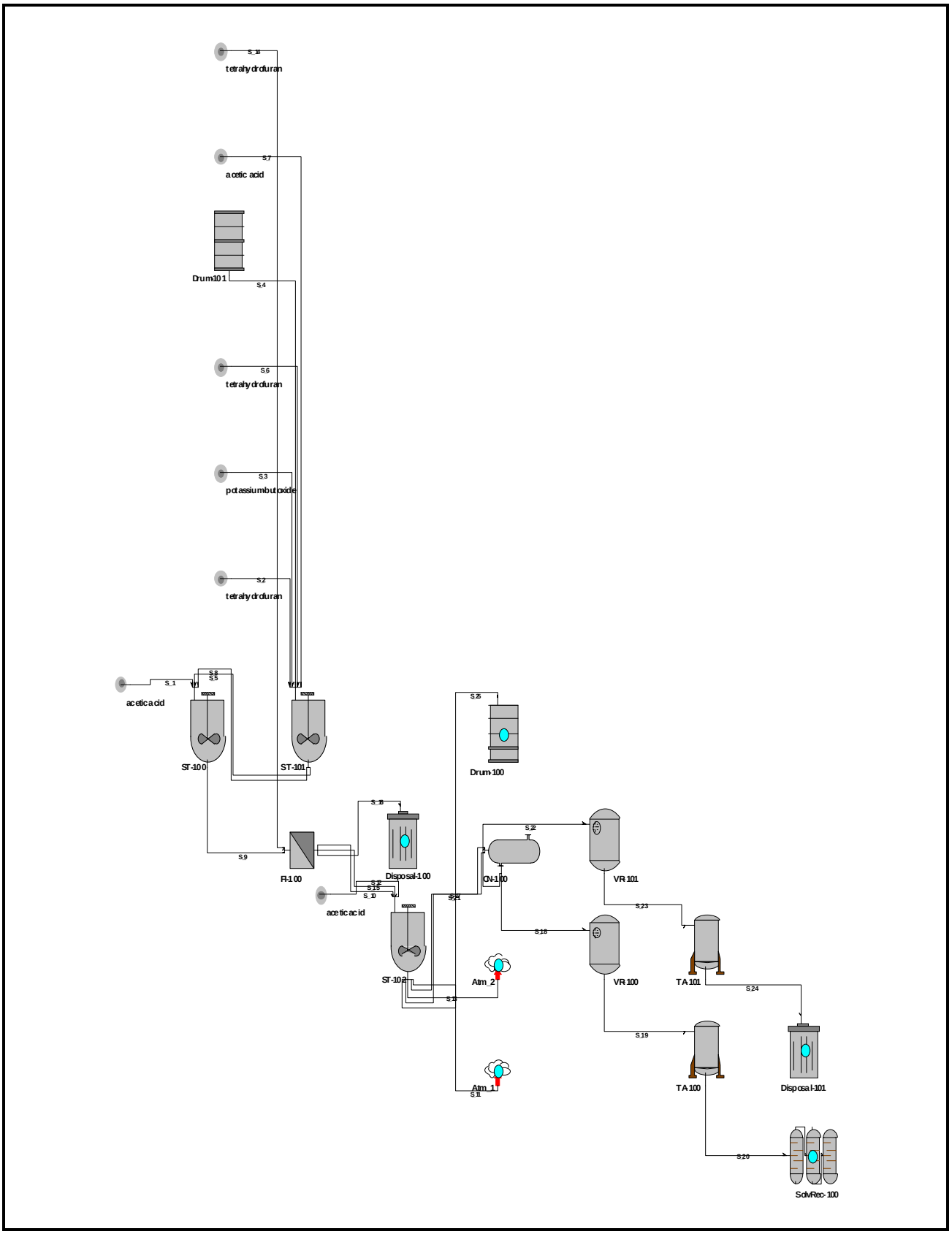
Step 1.20.	EVACUATE ST-102 to 7.333 kPa, operating 15 min, with condenser outlet temperature 20 ºC, send non condensed gas to Atm_1
Step 1.21.	CONCENTRATE batch in ST-102, using model Split with parameter(s): {separate material [18.4085 wt%, ACETIC ACID][1.5011 wt%, TERT-BUTYL-ALCOHOL][80.0904 wt%, TETRAHYDROFURAN] to Upper Layer}, naming the distillate as Distillate and sending distillate to receiver VR-100, through condenser CN-100 with outlet temperature 20 ºC
Step 1.22.	TRANSFER 100 wt% of the content of VR-100 to TA-100 , with condenser outlet temperature 20 ºC
Step 1.23.	TRANSFER 100 wt% of the content of TA-100 to SolvRec-100 , the transferred portion being named THF-ACOH-Dist, with condenser outlet temperature 20 ºC
Step 1.24.	SEQUENTIAL END
Step 1.25.	PARALLEL END
Step 1.26.	CHARGE 241 kg of ACETIC ACID to ST-102, with condenser outlet temperature 20 ºC
Step 1.27.	EVACUATE ST-102 to 2.000 kPa, operating 15 min, with condenser outlet temperature 20 ºC, send non condensed gas to Atm_2
Step 1.28.	CONCENTRATE batch in ST-102, using model Rayleigh distill with parameter(s): {distillate volume reaches 136.4 l,using ACETIC ACID as key compound}, naming the distillate as Distillate and sending distillate to receiver VR-101, through condenser CN-100 with outlet temperature 20 ºC
Step 1.29.	TRANSFER 100 wt% of the content of VR-101 to TA-101 , with condenser outlet temperature 20 ºC
Step 1.30.	TRANSFER 100 wt% of the content of TA-101 to Disposal-101 , the transferred portion being named ACOH-Dist, with condenser outlet temperature 20 ºC
Step 1.31.	TRANSFER 100 wt% of the content of ST-102 to Drum-100 , the transferred portion being named N-HYDROXY-SOLUTION

Table 1.6 shows a waste stream table of all the effluent streams included within this stage. Stream 16 is a THF wet cake, S_20 is a THF-ACOH distillate, S_24 is an ACOH distillate, and S_25 is n-hydroxy solution. Figure 1.3 is a thorough flowsheet of the complete process.

Table 6. Waste Stream Table of Stage 3 – N-HYDROXY

	S_16	S_20	S_24	S_25
ORIGIN	FI-100	TA-100	TA-101	ST-102
DESTINATION	Disposal-100	SolvRec-100	Disposal-101	Drum-100
TOTAL MASS (kg)	14.562	24.146	142.82	234.71
VOLUME (m^3)	0.010	0.023	0.136	0.213
DENSITY	1488.709	1049.009	1047.069	1101.978
TEMPERATURE (C)	25.000	20	20	24.315
PRESSURE (kPa)	101.325	101.325	101.325	101.325
PHASE	Solid	Liquid	Liquid	Liquid
COMPOSITION (kg per kg of batch)				
Tetrahydrofuran	2.912	0.000	0.000	0.000
Potassium-butoxide	2.233	0.000	0.000	0.000
Hydroxamine-iv	0.000	0.000	0.000	0.230
Acetic acid	0.000	24.039	142.820	204.705
n-hydroxy	0.000	0.000	0.000	22.769
tert-butyl-alcohol	0.000	0.107	0.000	7.006
Koac	9.417	0.000	0.000	0.000

Figure 3. Stage 3 – N-HYDROXY Process Flowsheet


tetrahydrofuran
acetic acid
Drum-101
potassiumbutoxide
tetrahydrofuran
acetic acid
ST-100
ST-101
Drum-100
Disposal-100
FI-100
CN-100
VR-101
acetic acid
ST-102
Atm_2
VR-100
TA-101
Atm_1
TA-100
Disposal-101
SolvRec-100

1.5. Stage 4—ACETATE-SALT Process Summary:

MK-VI-Acetate-Salt ($C_{18}H_{19}NO_2$) is produced from N-Hydroxy during this long series of steps. It begins with a purge of ST-100 (NOTE: This is a different tank than the ST-100 in Case 1. Although in each case the same name may appear for certain vessels as from other cases, each case was programmed separately and therefore is independent from any other case.) and a pressurization followed by the HYDROGENOLYSIS reaction. Afterwards, the batch is filtered, washed, evacuated, concentrated twice, extracted four times, filtered, washed, evacuated, concentrated, centrifuged, washed, and dried. The HYDROGENOLYSIS reaction is:

1 N-HYDROXY + 1 HYDROGEN + 1 ACETIC ACID -> 1 MK-VI-ACETATE-SALT + 1 WATER

The batch cycle time is 589.4 hours, and the batch recipe is shown in Table 1.7.

Table 7. Operating Steps for Stage 6 – MK-MALEATE

Step 1.	Start
Step 1.1.	CHARGE 140.9 l of N-HYDROXY-V-SOLUTION to ST-100, with condenser outlet temperature 20 ºC
Step 1.2.	CHARGE 140.9 l of WATER to ST-100, with condenser outlet temperature 20 ºC
Step 1.3.	CHARGE 4.700 kg of PALLADIUM-CATALYST to ST-100, with condenser outlet temperature 20 ºC
Step 1.4.	CHARGE 140.9 l of ETHANOL to ST-100, with condenser outlet temperature 20 ºC
Step 1.5.	PRESSURE PURGE ST-100 3 time(s) with NITROGEN, between high pressure 202.7 kPa, and low pressure 7.093 kPa, send gas to Atm-100, with condenser outlet temperature 20 ºC
Step 1.6.	PRESSURIZE ST-100 to pressure 377.1 kPa, with HYDROGEN, operating time 10 min
Step 1.7.	HEAT ST-100 to 50 ºC , with condenser outlet temperature 20 ºC
Step 1.8.	CHARGE 0.2000 kg of HYDROGEN to TA-100, with condenser outlet temperature 20 ºC
Step 1.9.	REACT in ST-100 isothermally, for 360 min, while adding 100 wt% of the content in TA-100, via [HYDROGENOLYSIS, Rank: 1, conversion: 98.00%, yield: 95.00%]
Step 1.10.	COOL ST-100 to 25 ºC
Step 1.11.	VENT ST-100, to Scrubber-100, giving the name Exhaust-gas, over 9 min
Step 1.12.	CHARGE 5 kg of Solca Floc to FI-100, with condenser outlet temperature 20 ºC
Step 1.13.	FILTER 100 wt% of batch from ST-100 in FI-100, separating materials [110.6 kg, ETHANOL][0.0194 kg, HYDROGEN][253.7 kg, N-HYDROXY-V-SOLUTION][0.0988 kg, NITROGEN][4.7 kg, PALLADIUM-CATALYST][140.1 kg, WATER], as solid, lod of cake 50 wt% liquid in total mass, sending mother liquor to ST-101 , giving the name Mother-Liquor, operating time 240 min, with condenser outlet temperature 20 ºC
Step 1.14.	WASH CAKE in FI-100 with 20.40 kg of WASH-34, sending wash to ST-101, name it Spent-wash, assume displacement, lod of cake 20 wt% liquid in total mass, number of washes 1, operating time 14400 min per wash
Step 1.15.	TRANSFER 100 wt% of the content of FI-100 to SolvRec-100 , the transferred portion being named Spent-Catalyst, with condenser outlet temperature 20 ºC
Step 1.16.	EVACUATE ST-101 to 6.666 kPa, operating 15 min, with condenser outlet temperature 20 ºC, send non condensed gas to Atm_1

Step 1.17.	CONCENTRATE batch in ST-101, using model Rayleigh distill with parameter(s): {distillate volume reaches 28 l,using ETHANOL as key compound}, using heating utility Super Heated Steam, naming the distillate as Distillate and sending distillate to receiver VR-100, through condenser CN-100 with outlet temperature 20 ºC
Step 1.18.	TRANSFER 100 wt% of the content of VR-100 to TA-101 , with condenser outlet temperature 20 ºC
Step 1.19.	TRANSFER 100 wt% of the content of TA-101 to Disposal-100 , the transferred portion being named ETOH-H2O-ACOH-Dist, with condenser outlet temperature 20 ºC
Step 1.20.	CHARGE 279.6 l of WATER to ST-101, with condenser outlet temperature 20 ºC
Step 1.21.	CONCENTRATE batch in ST-101, using model Rayleigh distill with parameter(s): {distillate volume reaches 140.9 l,using ETHANOL as key compound}, using heating utility Super Heated Steam, naming the distillate as Distillate and sending distillate to receiver VR-101, through condenser CN-100 with outlet temperature 20 ºC
Step 1.22.	TRANSFER 100 wt% of the content of VR-101 to TA-102 , with condenser outlet temperature 20 ºC
Step 1.23.	TRANSFER 100 wt% of the content of TA-102 to Disposal-101 , the transferred portion being named H2O-Dist, with condenser outlet temperature 20 ºC
Step 1.24.	VENT ST-101, to Atm-101, giving the name Exhaust-gas, over 9 min
Step 1.25.	CHARGE 140.9 l of WATER to ST-101, with condenser outlet temperature 20 ºC
Step 1.26.	CHARGE 20.20 kg of TOLUENE to ST-101, with condenser outlet temperature 20 ºC
Step 1.27.	TRANSFER 100 wt% of the content of ST-101 to EX-100 , with condenser outlet temperature 20 ºC
Step 1.28.	EXTRACT in EX-100, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-34-1}, sending bottom layer to ST-102, giving the name Bottom-Layer with condenser outlet temperature 20 ºC
Step 1.29.	TRANSFER 100 wt% of the content of EX-100 to TA-103 , with condenser outlet temperature 20 ºC
Step 1.30.	TRANSFER 100 wt% of the content of TA-103 to SolvRec-101 , the transferred portion being named toluene-waste-layer, with condenser outlet temperature 20 ºC
Step 1.31.	CHARGE 150.3 kg of ISOPROPYL ACETATE to ST-102, with condenser outlet temperature 20 ºC
Step 1.32.	COOL ST-102 to 10 ºC
Step 1.33.	CHARGE 41.90 kg of 15%AMMONIUM-HYDROXIDE to ST-102, over 30 min, with condenser outlet temperature 20 ºC
Step 1.34.	TRANSFER 100 wt% of the content of ST-102 to EX-101 , with condenser outlet temperature 20 ºC
Step 1.35.	EXTRACT in EX-101, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-34-op32}, sending bottom layer to EX-100, giving the name Botom-Layer with condenser outlet temperature 20 ºC
Step 1.36.	CHARGE 50.80 kg of ISOPROPYL ACETATE to EX-100, with condenser outlet temperature 20 ºC
Step 1.37.	EXTRACT in EX-100, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-34-op32}, sending bottom layer to TA-104, giving the name Bottom-Layer with condenser outlet temperature 20 ºC
Step 1.38.	TRANSFER 100 wt% of the content of TA-104 to Disposal-102 , the transferred portion being named AQ-NH4-Waste-Layer, with condenser outlet temperature 20 ºC
Note:	Combine the two organic layers
Step 1.39.	TRANSFER 100 wt% of the content of EX-100 to EX-101 , with condenser outlet temperature 20 ºC
Step 1.40.	CHARGE 69.70 kg of BBRINE to EX-101, with condenser outlet temperature 20 ºC
Step 1.41.	EXTRACT in EX-101, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-34-2}, sending bottom layer to TA-105, giving the name Bottom-Layer with condenser outlet temperature 20 ºC
Step 1.42.	TRANSFER 100 wt% of the content of EX-101 to ST-103 , with condenser outlet temperature 20 ºC
Step 1.43.	CHARGE 2.300 kg of CARBON to ST-103, with condenser outlet temperature 20 ºC
Step 1.44.	CHARGE 2 kg of SUPER-CEL to ST-103, with condenser outlet temperature 20 ºC

Step 1.45.	FILTER 100 wt% of batch from ST-103 in FI-101, separating materials [100.0000 wt%, CARBON][100.0000 wt%, SUPER-CEL], as solid, lod of cake 30 wt% liquid in total mass, sending mother liquor to ST-104 at final temperature 20 ºC, giving the name Mother-Liquor, operating time 240 min
Step 1.46.	WASH CAKE in FI-101 with 25.40 kg of ISOPROPYL ACETATE, sending wash to ST-104, name it Spent-wash, assume displacement, lod of cake 20 wt% liquid in total mass, number of washes 1, operating time 3600 min per wash
Step 1.47.	TRANSFER 100 wt% of the content of FI-101 to Disposal-104 , the transferred portion being named IPAC-Wet-Cake, with condenser outlet temperature 20 ºC
Step 1.48.	EVACUATE ST-104 to 2.000 kPa, operating 15 min, with condenser outlet temperature 20 ºC, send non condensed gas to Atm_2
Step 1.49.	CONCENTRATE batch in ST-104, using model Rayleigh distill with parameter(s): {distillate volume reaches 1 l,using ISOPROPYL ACETATE as key compound}, using heating utility Hot Water, naming the distillate as Distillate and sending distillate to receiver VR-102, through condenser CN-100 with outlet temperature 0 ºC
Step 1.50.	TRANSFER 100 wt% of the content of VR-102 to SolvRec-102 , the transferred portion being named IPAC-Dist, with condenser outlet temperature 20 ºC
Step 1.51.	VENT ST-104, to ATM-102, giving the name Exhaust-gas, over 9 min
Step 1.52.	CHARGE 230.3 kg of CYCLOHEXANE to ST-104, with condenser outlet temperature 20 ºC
Step 1.53.	CHARGE 7.300 kg of ACETIC ACID to ST-104, over 60 min, with condenser outlet temperature 20 ºC
Note:	Acetate-Salt crystallizes during addition
Step 1.54.	COOL ST-104 to 10 ºC
Step 1.55.	AGE ST-104, for 60 min, and maintain temperature
Step 1.56.	CENTRIFUGE 100 wt% of batch from ST-104 in CE-100 for 1 time(s), separating materials [98.0000 wt%, MK-VI-ACETATE-SALT] as solid, lod of cake 10 wt% liquid in total mass, sending mother-liquor to TA-106, cake stays in CE-100, total operation time 240 min, with condenser outlet temperature 20 ºC
Step 1.57.	WASH CAKE in CE-100 with 38.50 kg of CYCLOHEXANE, sending wash to TA-106, name it Spent-wash, assume displacement, lod of cake 20 wt% liquid in total mass, number of washes 1, operating time 14400 min per wash
Step 1.58.	TRANSFER 100 wt% of the content of TA-106 to SolvRec-103 , the transferred portion being named CYHX-IPAX-ACOH-ML+Wash, with condenser outlet temperature 20 ºC
Step 1.59.	TRANSFER 100 wt% of the content of CE-100 to DR-100 , with condenser outlet temperature 20 ºC
Step 1.60.	DRY in DR-100, at 25 ºC, for 480 min, sending vapor to Scrubber-101 , with loss on drying 0.3000 wt% liquid in total mass
Step 1.61.	TRANSFER 100 wt% of the content of DR-100 to Drum-100 , the transferred portion being named MK-VII-ACETATE-SALT-CRUDE

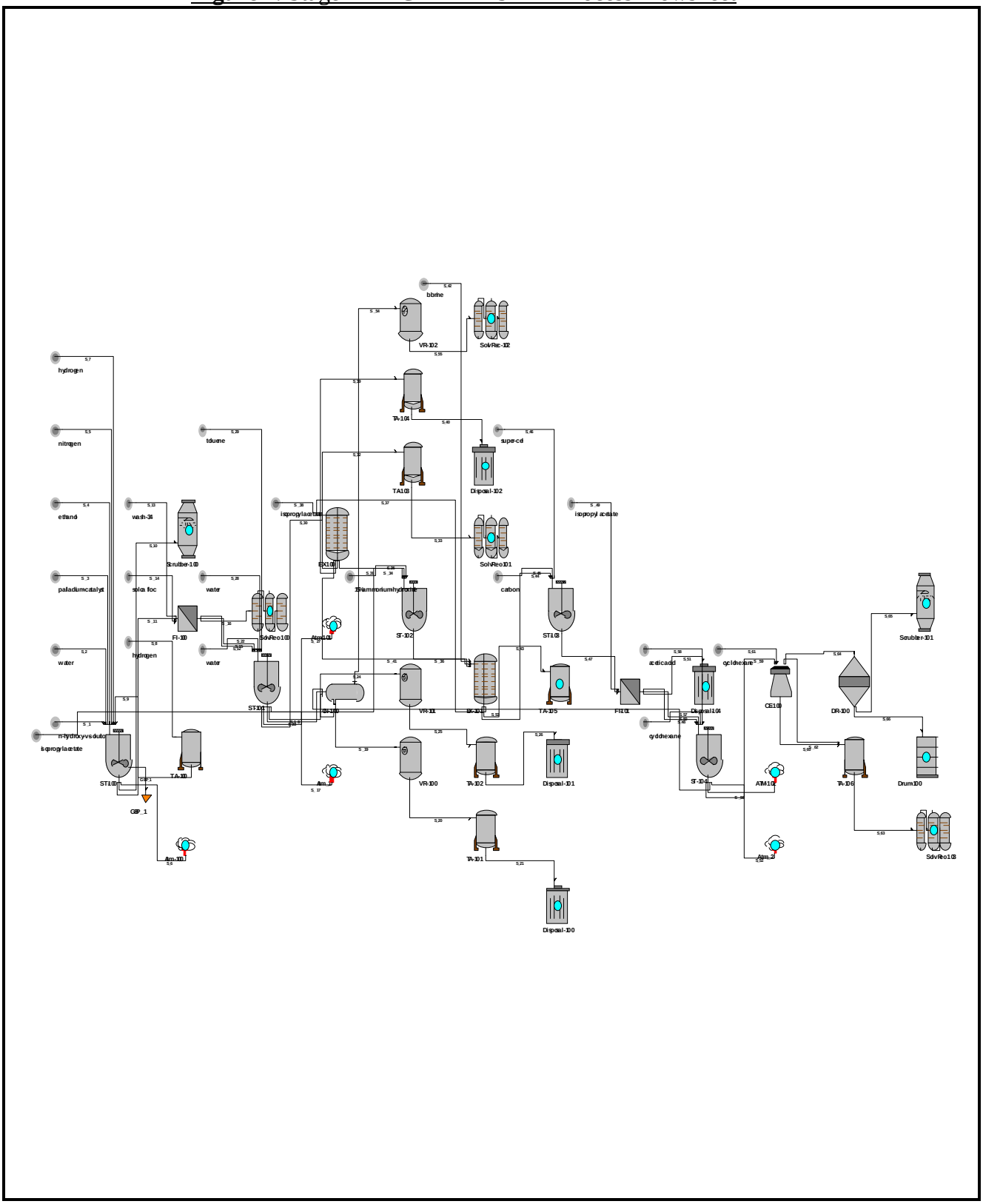
Table 1.8 shows a waste stream table of all the effluent streams included within this stage, and Figure 1.4 is a thorough flowsheet of the complete process. Stream 6 is a gas removed, S_16 is a solid spent-catalyst, S_21 is a liquid distillate containing ethanol and acetate, S_26 is a water distillate, S_33 is a liquid toluene waste layer, S_40 is a liquid aqueous ammonium waste layer, S_43 is a liquid bottom layer, S_51 is a solid isopropyl acetate wet cake, S_55 is an isopropyl acetate liquid distillate, S_63 is the mother liquor wash, and S_66 is the crude acetate salt.

Table 8. Waste Stream Table of Stage 4 – ACETATE SALT

	S_6	S_16	S_21	S_26	S_33	S_40	S_43
Origin	ST-100	FI-100	TA-101	TA-102	TA-103	TA-104	EX-101
Destination	Atm-100	SolvRec-100	Disposal-100	Disposal-101	SolvRec-101	Disposal-102	TA-105
Total Mass (kg)	3941.786	5.875	28.122	140.383	21.579	195.463	69.926
Volume (m^3)	0.387	0.004	0.028	0.141	0.024	0.192	0.057
Density (kg/m^3)	10196.734	1521.598	1004.368	996.338	894.117	1017.647	1235.863
Temperature (C)	25.000	25.000	20.000	20.000	25.000	13.620	16.986
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Gaseous	Solid	Liquid	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)							
acetic acid	109.109	0.438	12.738	0.094	0.000	0.168	0.000
n-hydroxy	0.000	0.000	0.000	0.000	0.656	0.000	0.000
tert-butyl-alcohol	0.000	0.000	0.000	0.000	0.000	8.207	0.000
Water	140.209	0.405	8.922	140.289	0.014	171.372	44.597
palladium-catalyst	0.000	4.700	0.000	0.000	0.000	0.000	0.000
Ethanol	110.764	0.333	5.437	0.000	0.000	0.000	0.000
Nitrogen	3581.704	0.000	0.857	0.000	0.000	0.000	0.000
Hydrogen	0.000	0.000	0.168	0.000	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	0.000	0.000	5.000	0.000
mk-vi-acetate-salt	0.000	0.000	0.000	0.000	0.710	0.004	0.036
Toluene	0.000	0.000	0.000	0.000	20.198	0.002	0.000
isopropyl acetate	0.000	0.000	0.000	0.000	0.000	0.006	0.201
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	10.706	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	25.092
Carbon	0.000	0.000	0.000	0.000	0.000	0.000	0.000
super-cel	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_51	S_55	S_63	S_66
Origin	FI-101	VR-102	TA-106	DR-100
Destination	Disposal-104	SolvRec-102	SolvRec-103	Drum-100
Total Mass (kg)	5.375	0.896	268.142	34.880
Volume (m^3)	0.003	0.001	0.338	0.019
Density (kg/m^3)	1595.446	896.331	794.344	1792.856
Temperature (C)	23.784	0.000	11.672	25.000
Pressure (kPa)	101.325	101.325	101.325	101.325
Phase	Solid	Liquid	Liquid	Solid
Composition (kg per kg batch)				
acetic acid	0.000	0.000	7.299	0.000
n-hydroxy	0.000	0.000	0.000	0.000
tert-butyl-alcohol	0.000	0.000	0.000	0.000
water	0.000	0.002	0.027	0.000
palladium-catalyst	0.000	0.000	0.000	0.000
ethanol	0.000	0.000	0.000	0.000
nitrogen	0.000	0.000	0.000	0.000
hydrogen	0.000	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	0.000
mk-vi-acetate-salt	0.000	0.000	0.711	34.775
toluene	0.000	0.000	0.000	0.000
Isopropyl acetate	1.075	0.894	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000
carbon	2.300	0.000	0.000	0.000
super-cel	2.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	260.106	0.105

Figure 4. Stage 4 – ACETATE SALT Process Flowsheet



1.6. Stage 5—L-MALEATE-SALT Process Summary:

Acetate-Salt-VI is the main raw material and Maleate-Salt-VII ($C_{22}H_{27}NO_6$) is the intermediate. Different than the previous cases, the reaction takes place halfway into the process rather than towards the beginning. First, two extractions are performed, then an evacuation, two concentrations, a pressurization, then the SALT-FORMATION reaction, a centrifuge, washing, and a second centrifuge and washing. This, however, did not succeed in my case study. An error in the reaction step that I was unable to find any solution for resulted in no data for this stage, but we will proceed forward and just state that the maleate salt is produced in this stage from acetate salt.

1.7. Stage 6—MK-MALEATE Process Summary:

The main product is made in this, the final process of the six, which is MK-VIII-Maleate. This begins with an extraction, then an evacuation, two concentration steps, a pressurization, an adiabatic reaction via SALT-FORMATION2, a centrifuge followed by two washes, and finally a drying. The SALT-FORMATION-2 reaction is:

1 L-MALATE-SALT-VII + 1 MALEIC ACID -> 1 MALEATE-VIII + 1 MALIC ACID + 1 ETHANOL

The batch cycle time is 296.9 hours, and the batch recipe is shown in Table 1.2.6.

Table 9. Operating Steps for Stage 6 – MK-MALEATE

Step 1.	Start
Step 1.1.	CHARGE 144.8 kg of METHYLENE-CHLORIDE to ST-100, with condenser outlet temperature 20 ºC
Step 1.2.	CHARGE 68.19 l of WATER to ST-100, with condenser outlet temperature 20 ºC
Step 1.3.	CHARGE 10.90 kg of L-MALATE-SALT-VII to ST-100, from Drum-100, with condenser outlet temperature 20 ºC
Step 1.4.	CHARGE 14.80 kg of 15%AMMONIUM-HYDROXIDE to ST-100, with condenser outlet temperature 20 ºC
Step 1.5.	AGE ST-100, for 30 min, and maintain temperature
Step 1.6.	TRANSFER 100 wt% of the content of ST-100 to EX-100 , with condenser outlet temperature 20 ºC
Step 1.7.	EXTRACT in EX-100, over 60 min, using model Extraction with parameter(s): {Extraction data EXDATA-36}, sending bottom layer to ST-101, giving the name Bottom-Layer with condenser outlet temperature 20 ºC
Step 1.8.	TRANSFER 100 wt% of the content of EX-100 to TA-100 , with condenser outlet temperature 20 ºC
Step 1.9.	TRANSFER 100 wt% of the content of TA-100 to Disposal-100 , the transferred portion being named AQ-NH4-Waste-Layer, with condenser outlet temperature 20 ºC
Step 1.10.	EVACUATE ST-101 to 7.333 kPa, operating 15 min, with condenser outlet temperature 20 ºC, send non condensed gas to Atm_1

Step 1.11.	CONCENTRATE batch in ST-101, using model Split with parameter(s): {separate material [25.0000 mole%, AMMONIUM HYDROXIDE][25.0000 mole%, L-MALATE-SALT-VII][25.0000 mole%, METHYLENE-HLORIDE][25.0000 mole%, WATER] to Upper Layer}, using heating utility Hot Water, naming the distillate as mec12-Dist and sending distillate to receiver VR-100, through condenser CN-100 with outlet temperature 20 ºC
Step 1.12.	TRANSFER 100 wt% of the content of VR-100 to TA-101 , with condenser outlet temperature 20 ºC
Step 1.13.	TRANSFER 100 wt% of the content of TA-101 to SolvRec-100 , the transferred portion being named MEC12-Dist, with condenser outlet temperature 20 ºC
Step 1.14.	CHARGE 37.60 kg of ETHANOL to ST-101, with condenser outlet temperature 20 ºC
Step 1.15.	CONCENTRATE batch in ST-101, using model Rayleigh distill with parameter(s): {distillate volume reaches 13.64 l,using ETHANOL as key compound}, using heating utility Hot Water, naming the distillate as ETOH-Dist and sending distillate to receiver VR-101, through condenser CN-100 with outlet temperature 20 ºC
Step 1.16.	PRESSURIZE ST-101 to pressure 101.3 kPa, with Nitrogen, operating time 10 min
Step 1.17.	TRANSFER 100 wt% of the content of VR-101 to TA-102 , with condenser outlet temperature 20 ºC
Step 1.18.	TRANSFER 100 wt% of the content of TA-102 to SolvRec-101 , the transferred portion being named ETOH-MEC12-Dist, with condenser outlet temperature 20 ºC
Step 1.19.	TRANSFER 100 wt% of the content of ST-101 to ST-102 , with condenser outlet temperature 20 ºC
Step 1.20.	CHARGE 11.20 kg of ethanol-maleic-acid-solution to TA-103, with condenser outlet temperature 20 ºC
Step 1.21.	REACT in ST-102 adiabatically, for 120 min, while adding 100 wt% of the content in TA-103, via [SALT-FORMATION2, Rank: 1, conversion: 95.00%, yield: 100.00%]
Step 1.22.	CHARGE 2.300 kg of MALEATE-VIII to ST-102, with condenser outlet temperature 20 ºC
Step 1.23.	CHARGE 5.600 l of ETHANOL to ST-102, with condenser outlet temperature 20 ºC
Step 1.24.	AGE ST-102, for 30 min, and maintain temperature
Step 1.25.	COOL ST-102 to 20 ºC
Step 1.26.	CHARGE 23.70 kg of ETHYL ACETATE to ST-102, with condenser outlet temperature 20 ºC
Step 1.27.	AGE ST-102, for 60 min, and maintain temperature
Step 1.28.	COOL ST-102 to 3 ºC, over 120 min
Step 1.29.	AGE ST-102, for 120 min, and maintain temperature
Step 1.30.	CENTRIFUGE 100 wt% of batch from ST-102 in CE-100 for 1 time(s), separating materials [99.0000 wt%, MALEATE-VIII] as solid, lod of cake 30 wt% liquid in total mass, sending mother-liquor to TA-104, cake stays in CE-100, total operation time 240 min, with condenser outlet temperature 20 ºC
Step 1.31.	WASH CAKE in CE-100 with 16.10 kg of ethanol-ethylacetate-solution, sending wash to TA-104, name it Spent-wash, assume displacement, lod of cake 20 wt% liquid in total mass, number of washes 1, operating time 14400 min per wash
Step 1.32.	CHARGE 16.10 kg of ethanol-ethylacetate-solution to ST-102, with condenser outlet temperature 20 ºC
Step 1.33.	COOL ST-102 to 2 ºC
Step 1.34.	WASH CAKE in CE-100 with 16.10 kg of ethanol-ethylacetate-solution, sending wash to TA-104, name it Spent-wash, assume displacement, lod of cake 30 wt% liquid in total mass, number of washes 1, operating time 1800 min per wash
Step 1.35.	TRANSFER 100 wt% of the content of TA-104 to SolvRec-102 , the transferred portion being named ETOAC-ETOH-ML+Wash, with condenser outlet temperature 20 ºC
Step 1.36.	TRANSFER 100 wt% of the content of CE-100 to DR-100 , with condenser outlet temperature 20 ºC
Step 1.37.	DRY in DR-100, at 25 ºC, for 720 min, sending vapor to Scrubber-100 , with loss on drying 0.10000 wt% liquid in total mass

Step 1.38.	TRANSFER 100 wt% of the content of DR-100 to Drum-101 , the transferred portion being named FINAL-PRODUCT

Table 1.12 shows a waste stream table of all the effluent streams included within this stage, and Figure 1.6 is a thorough flowsheet of the complete process. Stream 8 is an aqueous ammonium waste layer, S_13 is methylene chloride, S_19 is an ethyl alcohol-methylene chloride distillate, S_33 is the spent wash from Step 1.34 of this stage, and S_36 is actually the final product, in solid phase.

Table 10. Waste Stream Table of Stage 6 – MK-MALEATE

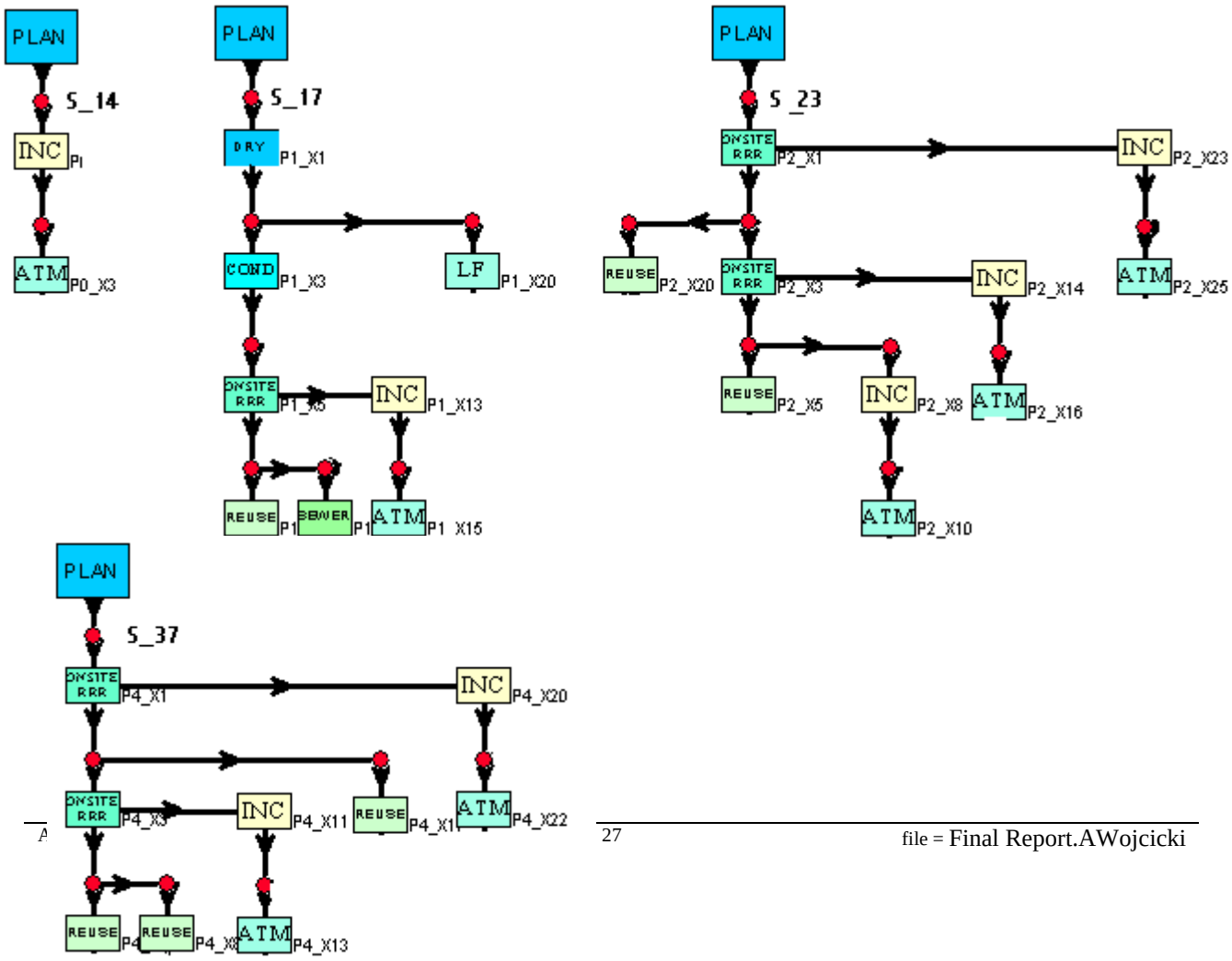
	S_8	S_13	S_19	S_33	S_36
Origin	TA-100	TA-101	TA-102	TA-104	DR-100
Destination	Disposal-100	SolvRec-100	SolvRec-101	SolvRec-102	Drum-101
Total Mass (kg)	79.044	38.915	10.882	413.961	8.683
Volume (m^3)	0.079	0.022	0.014	0.171	0.005
Density (kg/m^3)	996.435	1797.486	790.831	2425.709	1797.911
Temperature (C)	25.000	20	20	6.08	25
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Solid	Liquid	Gaseous	Solid
Composition (wt%)					
Methylene-chloride	0.145	36.164	0.000	108.491	0.000
Water	78.791	0.019	0.007	0.050	0.000
l-malate-salt-vii	0.108	2.698	0.000	0.406	0.000
Ammonium hydroxide	0.000	0.033	0.100	0.000	0.000
Ethanol	0.000	0.000	10.775	52.925	0.005
Nitrogen	0.000	0.000	0.000	209.088	0.000
Maleic acid	0.000	0.000	0.000	3.378	0.000
Maleate-viii	0.000	0.000	0.000	0.087	8.674
Malic acid	0.000	0.000	0.000	2.567	0.000
Ethyl acetate	0.000	0.000	0.000	36.967	0.004

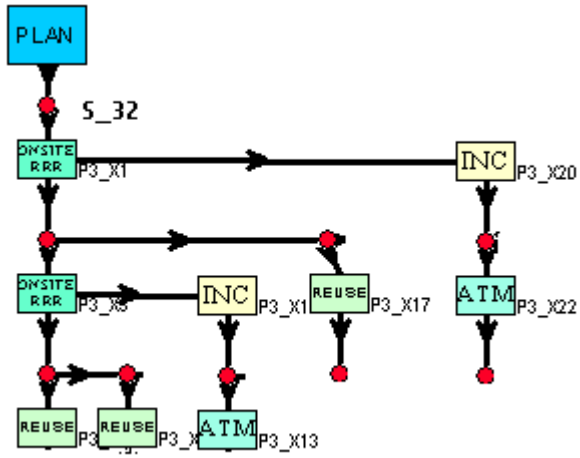
2. Management of Effluents in Recovery and Treatment

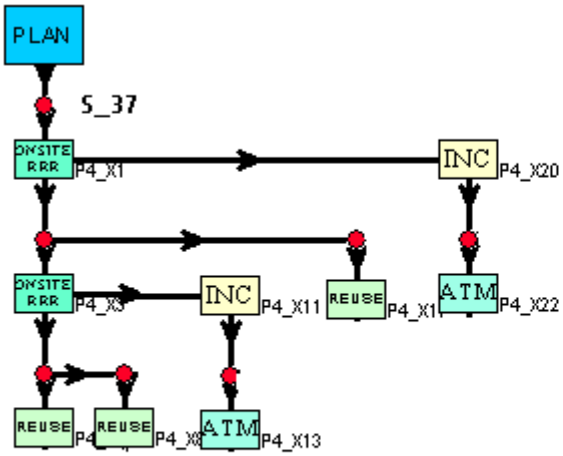
Several waste streams arise from each individual stage containing several organic impurities

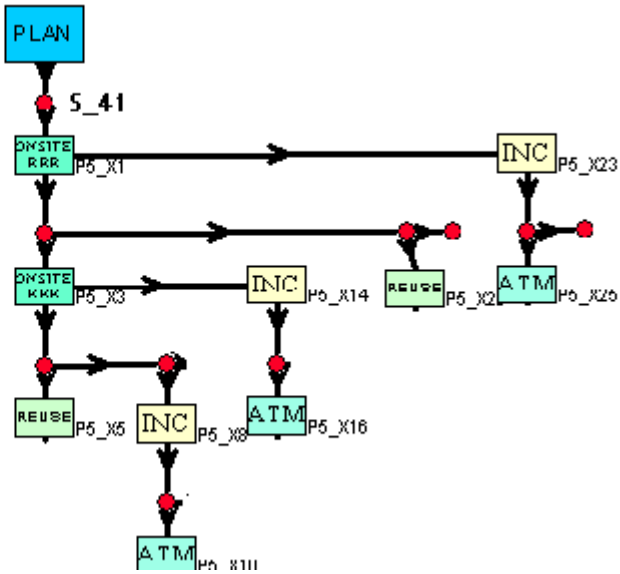
which must be sent to a treatment selector in order to properly dispose of these wastes. In our methodology, incineration is always the default option for hazardous waste streams with low volatility and/or high calorific value. Many times the residue that is acquired from incineration is rich in acidic gases, and therefore a postcombustion treatment option must also be instituted (e.g. scrubber). Biological treatment and wet air oxidation are not very common options in this study since the majority of our waste streams have a very high organic content. The first production stage contains seven waste streams, and those streams were all sent to a colleague's selector program.My case study obviously produced numerous amounts of waste streams, and I sent the six waste streams of the first production stage to Mr. Aninda Chakraborty's waste treatment selector program. Figure 1.7 shows the outcome of each of the streams. As one can clearly see, incineration is indeed a default method and is present in each and every one of the policy trees. In some plans, only one path may be feasible, yet on others several options exist.

Figure 5. Waste Treatment Selector Program Applied to Stage 1









2.1. Superstructure Discussion

For the first waste stream, S_14, the only path that is considered is one in which the aqueous organic mixture is burned since there are too many solids, the mixture is not dilute enough for waste water treatment, yet not concentrated enough for solvent recovery. Stream S_17 consists of an almost completely solid cake of sodium chloride with trace amounts of organic and aqueous impurities. This stream is first sent to a dryer, where afterwards the solids are sent to a landfill for final disposal and the organics are sent to a condenser. Onsite recovery is implemented since there is a high enough concentration of solvents to be reused (the trace water goes into the sewer for final disposal). However, since the materials all come from a dirty

piece of solid cake, incineration is also an option which may actually, and this should always be considered, be less expensive than the recovery options. The next four waste streams are all similar in that they all contain mostly cyclohexane. Stream S_23 has little water, and everything can be burned to begin with or sent to recovery. The carbinol and THF can be recovered, and the half-organic-half-water mixture at the end can be sent to be burned. For S_32, the waste is about three-fourths cyclohexane and one-fourth THF with trace amounts of water and organics. The stream is sent to recovery for the cyclohexane and then again to recover the solvent THF. As always, the streams can be sent to burn at any time if it proves to be the better option. The organics, of course, are sent to be destroyed at the end to incineration. The last two streams resemble the previous one greatly, so further discussion is not necessary. The main idea one should take away with this is the methodology of how waste streams are treated by this automated program that is created by a human and made to think reasonably like one in order to choose the best option for each stream.

3. Detailed Chemistry of Combustion:

Coming into this project, the current incinerator model contained thorough carbon, hydrogen, nitrogen, and some halide chemistry along with the postcombustion treatment selector for any nitric oxide that may be produced. Over the ten weeks, I was able to add some more detail to the model by suggesting and committing to a sulfur combustion pathway and the different routes certain heavy metals take through incineration. Table X in Appendix A shows an example of how the current incinerator code is programmed and the functions that it can output from an incinerator feed.

3.1. Sulfur Chemistry

Bong-Mann Kim of the South Coast Air Quality Management District was able to inform me of the average split ratio of SO_2:SO_3 via email. The ratio that he proposed agreed with a few of my other sources, which is 97:3 (SO_2:SO_3). Essentially, all of the sulfur which enters the incinerator will exit as sulfur dioxide, a very harmful air pollutant which must go through postcombustion treatment in order to breakdown the potentially toxic molecule. The treatment selector that we have instituted as a result of much research on the web is a wet lime scrubber,

where a calcium hydroxide slurry is used in order for the sulfur dioxide to absorb into the rinse and precipitate as wet calcium sulfite, which can then be converted to almost pure gypsum.

Reasons for implementing a wet lime scrubber over a regular limestone scrubber include factors such as cost, efficiency, and maintenance. Overall, a wet lime scrubber has several advantages over a limestone scrubber. The following are some pro's to lime scrubbing technology: lime is more reactive and does not require a high temperature or heat of reaction; a lime scrubber requires less capital equipment and less maintenance on account of fewer pumps needed to run a cycle; the lime process has a 99% sulfur dioxide removal capability versus 95% by that of a limestone scrubber; lime systems require a relatively small volume of slurry—only three to five liters per cubic meter of gas ([21 to 45] gal/1000 cubic feet) to achieve 95% sulfur dioxide removal, versus at least fifteen liters of slurry per cubic meter of gas (110 gal/1000 cubic feet) that it would take for a limestone system to achieve 95% removal efficiency; the lime process uses about 0.8 to 1.3 percent of a power station's gross generation versus about 1.5 to 2.5 percent for a limestone process; the gypsum produced from a lime process is 97 to 99 percent pure, bright-white, and capable of being dewatered to less then ten percent moisture, whereas gypsum as a byproduct from the limestone process is only 90 to 95 percent pure, brownish or tan in color, and can only be dewatered to about ten to fifteen percent moisture content; the ability to remove 99% of sulfur dioxide with a lime scrubbing system allows power generators to retain valuable sulfur dioxide allowances rather than emit them, which can then sold from anywhere in between one to two hundred dollars per allowance; more valuable resources such as these allowances can be retained from a lime system; and lime scrubbing is often more cost-effective than burning low sulfur containing coal in the first place.

The system itself operates by a simple series of steps. First, lime is added to water in a tank where a quick reaction takes place and calcium hydroxide is formed. The resulting slurry is sprayed into the scrubber tower where it meets with the incoming gas that enters from the bottom of the cylinder. The sulfur dioxide is absorbed into the slurry as it flows upward and then precipitates as wet calcium sulfite (which can then be converted to gypsum). This technique is also a primary use for magnesium-enhanced lime (containing three to eight percent magnesium oxide), which provides high alkalinity that increases sulfur dioxide removal capacity and reduces scaling potential.

3.2. Heavy Metals

The metals that we are considering in this research are arsenic, beryllium, cadmium, chromium, copper, iron, lead, mercury, nickel, and zinc. As these elements enter the incinerator operating at approximately 1700 degrees Celsius, they will all oxidize and exit the unit either through the gas or solid residue stream. Beryllium, copper, iron, lead, nickel, and zinc will exit with the solid residue. Arsenic, cadmium, and mercury will exit with the gas residue stream. Chromium will go to the solid residue as Cr_2O_3 and to the gas residue as CrO_2 and CrO_3. Note, however, that although we may know that these metals will oxidize and enter one of the two exit streams, we do not know the split ratios of each of the metals' possible oxides.

4. Conclusion/Significance:

The scope of this project dealt with batch processes—processes which undergraduate chemical engineering students don't encounter much during their course study. Analyzing the complex chemistry involved in producing carbinol from trienone, and also having to deal with the undesired solid gel that must be quenched and broken, is enough to see the difference in between a batch process and a continuous process. The vessels and storage tanks I used throughout my case study were used for any various number of operations, unlike in a continuous process where each tank has a specific function each and every time a process is run.

The case study was a good experience for me in working with another simulation software package—Batch Design Kit. I have only worked with HYSYS before, and the BDK, although it may have contained a few bugs in each stage, I still feel it is a very powerful tool, especially for those who want to plan any kind of batch process and not have to go out and buy a plant just to see if it works. It also saves the user an enormous amount of labor if he or she were to do these operations by hand and calculate each and every stream by the same method. I give my recommendation to institute this program as part of a senior design class, perhaps, with a stronger emphasis on batch processes for a change.

The incinerator model took me a longer time to get started on, mainly because the information I was seeking was hard to find, no matter what I used as my resource. However, halfway into the program I was able to finally receive some help as to the fate of sulfur as it

enters an incinerator unit operating at 1700 degrees Celsius. Aninda Chakraborty's reasoning was proven correct by the information Bong-Mann Kim sent to me via email—all the sulfur that enters basically exits as sulfur dioxide.

One of the most important things I will take with me from this research experience is a higher degree of professionalism. I was given the opportunities to witness first hand how talks, theses, etc. are and should be presented. I was also in a different position at the table this time around as a pose to last summer, which found me being on the "seller" side while working as a co-op for BMW Manufacturing Company. This year, I knew what it was like to try and sell something, and also found very quickly that an idea, rather than a tangible object, is harder to market.

References

Castaldini, C., H.K. Willard, C.D. Wolbach, and L.R. Waterland, *Disposal of Hazardous Wastes in Industrial Boilers and Furnaces*, Noyes Publications, New Jersey, 1986.

Corey, Richard C., Editor, *Principles and Practices of Incineration*, Wiley-Interscience, New York, 1969.

de Nevers, Noel, *Air Pollution Control Engineering (Second Edition)*, McGraw Hill.

Using Lime for Flue Gas Scrubbing A Proven Solution!, http://www.lime.org/FGDfinal.pdf.

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APPENDIX A

In Table X, the first series of steps gets the amount of moles of each element (carbon, hydrogen, oxygen, nitrogen, and chloride) contained in the task mixture entering the incinerator unit. The reason for this is since this is an elemental balance that is concerned just with the atoms, not with what molecules are entering.

The carbon chemistry sets a 1:1 ratio for the amount of carbon dioxide formed from the number of carbon atoms that enter.

The water chemistry is a little more complicated here, since all of the hydrogen may not go to producing water vapor if chlorine atoms are present as well. Normally, for every hydrogen atom, half a water molecule is formed if there is no chlorine present. Since the amount of hydrogen chloride formed through incineration to the amount of chlorine entering is also a 1:1 ratio, the code is written so as to subtract the number of chlorine atoms from the number of hydrogen atoms, and then the result is halved in order to give the number of water molecules formed.

The nitrogen chemistry is also more than just a one line procedure. NO to NO_2 is formed in a 9:1 ratio. Ten percent of the number of nitrogen atoms entering is taken and the product is the number of NO_2 atoms in the flue gas. The number of NO atoms is equal then to the number of NO_2 atoms subtracted from the number of nitrogen atoms.

The oxygen demand is calculated through a formula that doubles the amount of carbon atoms in the mixture feed, adds it to half the quantity of {hydrogen atoms - chorine atoms}, the subtotal is then added to the number of NO atoms formed plus twice that of the number of NO_2 atoms formed, and finally the amount of oxygen already contained in the task mixture is subtracted from the previous total.

Table X: Partial Code for the Oxidize Procedure:

```
ACremain := aC.getCopy;
  Result := 0.;
  if not aC.isOxidizable then begin
    aResidue.addCompound(aCRemain);
    result := 0.;
    exit;
  end;
  aCBurnt := aC.getCopy;
  aCburnt.setMass(aC.getMass * eta);
  aCremain.setMass(aC.getMass * ( 1. - eta)); // what remains from compound;
  // teh burnt products
  c  := aCburnt.getMolesofElement('C');
```

```
h  := aCburnt.getMolesofElement('H');
o  := aCburnt.getMolesofElement('O');
n  := aCburnt.getMolesofElement('N');
cl := aCburnt.getMolesofElement('Cl');
// carbon chemistry
aC2 := TCompound.GetNew('CARBON DIOXIDE', 1);
aC2.SetMoles(c);
aResidue.addCompound(aC2);
// water chemistry
aC2 := TCompound.GetNew('WATER' ,  1);
aC2.SetMoles( (h - cl)/ 2. );
aC2.SetState(gaseous);
aResidue.addCompound(aC2);
// hcl chemistry
aC2 := TCompound.GetNew('HYDROGEN CHLORIDE', 1);
aC2.SetMoles(cl);
aResidue.addCompound(aC2);
// Lin/Cha 6-12-98
// nitrogen chemistry
no2 := 0.1 * n;  // 10% NO2 typically in the flue gas
no  := n - no2;
aC2 := Tcompound.GetNew('NITRIC OXIDE', 1);
aC2.SetMoles(no);
aResidue.addCompound(aC2);
aC2 := Tcompound.GetNew('NITROGEN DIOXIDE', 1);
aC2.SetMoles(no2);
aResidue.addCompound(aC2);
 // oxygen demand
o := 2 * c + (h - cl) / 2. + no + 2 * no2 - o; // no oxigen for the h in hcl
aResidue.addCompound(aCremain);
aTreated.addCompound(aCburnt);
result := o;
```

Table A.1. Total Stream Table for Stage 1 – GRIGNARD

	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8
Origin	Storage	Storage	Storage	Storage	Storage	Storage	Storage	ST-103
Destination	ST-100	ST-100	ST-100	ST-101	ST-101	ST-102	ST-102	CN-100
Total Mass (kg)	111.000	20.000	14.600	44.400	24.250	55.500	61.300	53.126
Volume (m^3)	0.112	0.013	0.014	0.050	0.013	0.063	0.034	0.060
Density (kg/m^3)	995.011	1522.969	1042.013	879.978	1800.000	879.978	1800.000	884.176
Temperature (C)	25.000	25.000	25.000	25.000	25.000	25.000	25.000	21.054
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	18.000
Phase	Liquid	Solid	Liquid	Liquid	Solid	Liquid	Solid	Gaseous
Composition (kg per kg batch)								
Water	111.000	0.000	0.000	0.000	0.000	0.000	0.000	0.006
sodium acetate	0.000	20.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.000	0.000	14.600	0.000	0.000	0.000	0.000	0.000
Tatrahydrofuran	0.000	0.000	0.000	44.400	0.000	55.500	0.000	53.120
Trienone	0.000	0.000	0.000	0.000	24.250	0.000	0.000	0.000
ether-3M	0.000	0.000	0.000	0.000	0.000	0.000	29.504	0.000
MEMGBR	0.000	0.000	0.000	0.000	0.000	0.000	31.796	0.000
Carbinol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Magnesium bromide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Magnesium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Acetic anhydride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_9	S_10	S_11	S_12	S_13	S_14	S_15	S_16
Origin	ST-101	Storage	ST-102	ST-100	EX-100	TA-100	Storage	EX-100
Destination	ST-102	ST-102	ST-100	EX-100	TA-100	Disposal-100	EX-100	TA-101
Total Mass (kg)	68.650	44.400	44.400	373.894	204.340	204.340	62.500	68.659
Volume (m^3)	0.064	0.050	0.050	0.340	0.165	0.165	0.029	0.035
Density (kg/m^3)	1078.962	879.978	885.278	1098.118	1235.982	1235.982	2160.286	1943.117
Temperature (C)	20.000	25.000	20.000	10.984	10.984	10.984	25.000	20.000
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Solid	Solid
Composition (kg per kg batch)								
Water	0.000	0.000	0.000	111.002	107.767	107.767	0.000	3.139
sodium acetate	0.000	0.000	0.000	20.000	20.001	20.001	0.000	0.000
acetic acid	0.000	0.000	0.000	0.621	0.619	0.619	0.000	0.000
Tatrahydrofuran	44.400	44.400	44.400	144.301	2.830	2.830	0.000	2.774
Trienone	24.250	0.000	0.000	0.243	0.243	0.243	0.000	0.000
ether-3M	0.000	0.000	0.000	29.504	29.505	29.505	0.000	0.000
MEMGBR	0.000	0.000	0.000	17.917	17.917	17.917	0.000	0.000
Carbinol	0.000	0.000	0.000	25.100	0.249	0.249	0.000	0.246
magnesium bromide	0.000	0.000	0.000	10.394	10.395	10.395	0.000	0.000
magnesium hydroxide	0.000	0.000	0.000	3.294	3.292	3.292	0.000	0.000
acetic anhydride	0.000	0.000	0.000	11.527	11.527	11.527	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	62.500	62.500
Cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_17	S_18	S_19	S_20	S_21	S_22	S_23	S_24
Origin	TA-101	ST-102	EX-100	ST-103	CN-100	ST-103	VR-100	Storage
Destination	Disposal-101	ST-100	ST-103	Atm_1	VR-100	CE-100	SolvRec-100	ST-103
Total Mass (kg)	68.650	185.450	163.395	0.887	53.126	734.288	53.126	175.732
Volume (m^3)	0.035	0.159	0.170	0.001	0.060	0.909	0.060	0.227
Density (kg/m^3)	1943.117	1163.573	958.701	885.287	885.289	807.708	885.289	773.109
Temperature (C)	20.000	12.500	20.000	20.000	20.000	10.000	20.000	25.000
Pressure (kPa)	101.325	101.325	101.325	18.000	101.325	18.000	101.325	101.325
Phase	Solid	Liquid	Liquid	Gaseous	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)								
water	3.139	0.000	0.095	0.000	0.006	0.081	0.006	0.000
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tatrahydrofuran	2.774	99.900	138.696	0.887	53.120	45.107	53.120	0.000
trienone	0.000	24.249	0.000	0.000	0.000	0.000	0.000	0.000
ether-3M	0.000	29.503	0.000	0.000	0.000	0.000	0.000	0.000
MEMGBR	0.000	31.795	0.000	0.000	0.000	0.000	0.000	0.000
carbinol	0.246	0.000	24.604	0.000	0.000	24.606	0.000	0.000
magnesium bromide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
magnesium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic anhydride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	62.500	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	664.494	0.000	175.732

	S_25	S_26	S_27	S_28	S_29	S_30	S_31	S_32
Origin	ST-103	CN-100	VR-101	Storage	ST-103	CN-100	VR-102	TA-102
Destination	CN-100	VR-101	TA-102	ST-103	CN-100	VR-102	TA-102	SolvRec-101
Total Mass (kg)	49.220	49.220	49.220	175.732	48.042	48.042	48.042	97.262
Volume (m^3)	0.061	0.060	0.060	0.227	0.061	0.060	0.060	0.120
Density (kg/m^3)	812.770	820.201	820.201	773.109	791.517	800.574	800.574	810.388
Temperature (C)	20.000	12.500	20.000	20.000	20.000	10.000	20.000	20.000
Pressure (kPa)	101.325	101.325	101.325	18.000	101.325	18.000	101.325	101.325
Phase	Gaseous	Liquid	Liquid	Liquid	Gaseous	Liquid	Liquid	Liquid
Composition (kg per kg batch)								
water	0.004	0.004	0.004	0.000	0.002	0.002	0.002	0.007
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tatrahydrofuran	21.020	21.020	21.020	0.000	11.341	11.341	11.341	32.361
trienone	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ether-3M	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MEMGBR	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbinol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
magnesium bromide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
magnesium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic anhydride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	28.196	28.196	28.196	175.732	36.698	36.698	36.698	64.894

	S_33	S_34	S_35	S_36	S_37	S_38	S_39	S_41
Origin	Storage	ST-103	CN-100	VR-103	TA-103	Storage	CE-100	TA-104
Destination	ST-103	CN-100	VR-103	TA-103	SolvRec-102	ST-103	TA-104	SolvRec-103
Total Mass (kg)	175.732	47.540	47.540	47.540	47.540	242.510	707.766	707.766
Volume (m^3)	0.227	0.061	0.060	0.060	0.060	0.314	0.892	0.892
Density (kg/m^3)	773.109	782.481	792.213	792.213	792.213	773.109	793.023	793.023
Temperature (C)	25.000	30.591	20.000	20.000	20.000	25.000	10.000	10.000
Pressure (kPa)	101.325	18.000	101.325	18.000	101.325	101.325	18.000	101.325
Phase	Liquid	Gaseous	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)								
water	0.000	0.002	0.002	0.002	0.002	0.000	0.078	0.078
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tatrahydrofuran	0.000	7.283	7.283	7.283	7.283	0.000	44.943	44.943
trienone	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ether-3M	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MEMGBR	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbinol	0.000	0.000	0.000	0.000	0.000	0.000	0.736	0.736
magnesium bromide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
magnesium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic anhydride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	175.732	40.263	40.263	40.263	40.263	242.510	662.009	662.009

	S_42	S_43	S_44
Origin	CE-100	DR-100	DR-100
Destination	DR-100	Scrubber-100	Drum-100
Total Mass (kg)	26.518	2.628	23.890
Volume (m^3)	0.017	0.003	0.013
Density (kg/m^3)	1597.002	779.143	1797.645
Temperature (C)	10.000	25.000	25.000
Pressure (kPa)	101.325	101.325	101.325
Phase	Solid	Gaseous	Solid
Composition (kg per kg batch)			
water	0.000	0.000	0.000
sodium acetate	0.000	0.000	0.000
acetic acid	0.000	0.000	0.000
tatrahydrofuran	0.169	0.167	0.001
trienone	0.000	0.000	0.000
ether-3M	0.000	0.000	0.000
MEMGBR	0.000	0.000	0.000
carbinol	23.866	0.000	23.866
magnesium bromide	0.000	0.000	0.000
magnesium hydroxide	0.000	0.000	0.000
acetic anhydride	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000
cyclohexane	2.483	2.461	0.022

Table A.2. Total Stream Table of Stage 2 – HYDROXYAMINATION

	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8
Origin	Storage	Storage	Storage	Storage	Storage	Storage	Storage	Drum-100
Destination	ST-100	ST-100	ST-100	ST-100	ST-100	TA-100	TA-100	TA-100
Total Mass (kg)	44.4	187.8	29.5	34.7	55.2	125.1	7.4	23.6
Volume (m^3)	0.025	0.104	0.016	0.023	0.036	0.069	0.004	0.013
Density (kg/m^3)	1800	1800	1800	1522.969	1553.325	1800	1800	1800
Temperature (C)	25	25	25	25	25	25	25	25
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Solid	Solid	Solid	Solid	Liquid	Solid	Solid	Solid
Composition (kg per kg batch)								
acetone-nitrile	44.400	0.000	0.000	0.000	0.000	0.000	7.400	0.000
methylene chloride	0.000	187.800	0.000	0.000	0.000	125.100	0.000	0.000
hydroxylamine-hydrochloride	0.000	0.000	29.500	0.000	0.000	0.000	0.000	0.000
sodium acetate	0.000	0.000	0.000	34.700	0.000	0.000	0.000	0.000
dichloroacetic acid	0.000	0.000	0.000	0.000	55.200	0.000	0.000	0.000
carbinol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	23.600
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hydroxylamine	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hydroxamine	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ammonium-dichloroacetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ammonium acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_9	S_10	S_11	S_12	S_14	S_39	S_13	S_15	S_16
Origin	TA-100	Storage	TA-100	Storage	TA-101	Storage	ST-100	EX-100	EX-100
Destination	ST-100	TA-100	ST-100	TA-101	ST-100	ST-100	EX-100	EX-101	TA-102
Total Mass (kg)	156.1	31.3	31.3	221.8	221.8	46	796.843	485.887	310.955
Volume (m^3)	0.087	0.017	0.017	0.234	0.234	0.044	0.588	0.303	0.285
Density (kg/m^3)	1800	1800	1800	947.574	947.574	1042.013	1355.077	1603.946	1090.65
Temperature (C)	25	25	25	25	25	25	15.841	15.841	15.841
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Solid	Solid	Solid	Liquid	Liquid	Liquid	Solid	Solid	Liquid
Composition (kg per kg batch)									
acetone-nitrile	7.401	0.000	0.000	0.000	0.000	0.000	51.803	51.800	0.000
methylene chloride	125.100	31.300	31.300	0.000	0.000	0.000	344.196	343.857	0.345
hydroxylamine-hydrochloride	0.000	0.000	0.000	0.000	0.000	0.000	0.104	0.107	0.000
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
dichloroacetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbinol	23.601	0.000	0.000	0.000	0.000	0.000	0.239	0.233	0.000
ammonium hydroxide	0.000	0.000	0.000	56.668	56.668	0.000	0.000	0.000	0.000
water	0.000	0.000	0.000	165.132	165.132	0.000	196.119	0.782	195.336
acetic acid	0.000	0.000	0.000	0.000	0.000	46.000	0.008	0.010	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	24.718	0.243	24.475
hydroxylamine	0.000	0.000	0.000	0.000	0.000	0.000	10.502	10.447	0.053
hydroxamine	0.000	0.000	0.000	0.000	0.000	0.000	24.447	24.430	0.012
ammonium-dichloroacetate	0.000	0.000	0.000	0.000	0.000	0.000	53.070	53.069	0.000
ammonium acetate	0.000	0.000	0.000	0.000	0.000	0.000	91.637	0.909	90.734
Cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_17	S_18	S_19	S_20	S_21	S_22	S_23	S_24
Origin	TA-102	Storage	EX-101	EX-101	TA-103	ST-101	ST-101	CN-100
Destination	Disposal-100	EX-101	ST-101	TA-103	Disposal-101	Atm_1	CN-100	VR-100
Total Mass (kg)	310.955	141.3	484.958	142.229	142.229	0.01	9.572	9.572
Volume (m^3)	0.285	0.065	0.302	0.067	0.067	0	0.039	0.035
Density (kg/m^3)	1090.65	2160.286	1608.158	2130.227	2130.227	1030.002	246.313	273.5
Temperature (C)	15.841	25	19.547	19.547	19.547	20	47.305	20
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	6.666	6.666	101.325
Phase	Liquid	Solid	Solid	Solid	Solid	Gaseous	Gaseous	Solid
Composition (kg per kg batch)								
acetone-nitrile	0.000	0.000	51.798	0.000	0.000	0.000	0.000	0.000
methylene chloride	0.345	0.000	343.510	0.344	0.344	0.000	0.000	0.000
hydroxylamine-hydrochloride	0.000	0.000	0.107	0.000	0.000	0.000	0.000	0.000
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
dichloroacetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbinol	0.000	0.000	0.233	0.001	0.001	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	195.336	0.000	0.005	0.778	0.778	0.003	0.000	0.000
acetic acid	0.000	0.000	0.010	0.000	0.000	0.007	0.002	0.002
sodium chloride	24.475	141.300	1.402	140.144	140.144	0.000	0.000	0.000
hydroxylamine	0.053	0.000	10.397	0.053	0.053	0.000	9.561	9.561
hydroxamine	0.012	0.000	24.418	0.013	0.013	0.000	0.000	0.000
ammonium-dichloroacetate	0.000	0.000	53.069	0.000	0.000	0.000	0.000	0.000
ammonium acetate	90.734	0.000	0.010	0.899	0.899	0.000	0.009	0.009
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_25	S_26	S_27	S_28	S_29	S_30	S_31	S_32
Origin	VR-100	Storage	ST-101	CN-100	VR-101	Storage	ST-101	CE-100
Destination	SolvRec-100	ST-101	CN-100	VR-101	SolvRec-101	ST-101	CE-100	TA-104
Total Mass (kg)	9.572	92	92.789	92.789	92.789	108.954	583.541	557.223
Volume (m^3)	0.035	0.119	0.003	0.12	0.12	0.141	0.402	0.386
Density (kg/m^3)	273.5	773.109	28669.283	773.231	773.231	773.109	1451.365	1445.224
Temperature (C)	20	25	67.647	11	11	25	9	9
Pressure (kPa)	101.325	101.325	6.666	101.325	101.325	101.325	6.666	6.666
Phase	Solid	Liquid	Gaseous	Liquid	Liquid	Liquid	Solid	Solid
Composition (kg per kg batch)								
acetone-nitrile	0.000	0.000	0.000	0.000	0.000	0.000	51.801	51.799
methylene chloride	0.000	0.000	0.000	0.000	0.000	0.000	343.513	343.511
hydroxylamine-hydrochloride	0.000	0.000	0.000	0.000	0.000	0.000	0.105	0.106
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
dichloroacetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbinol	0.000	0.000	0.000	0.000	0.000	0.000	0.233	0.234
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	1.400	1.404
hydroxylamine	9.561	0.000	0.789	0.789	0.789	0.000	0.047	0.045
hydroxamine	0.000	0.000	0.000	0.000	0.000	0.000	24.421	0.730
ammonium-dichloroacetate	0.000	0.000	0.000	0.000	0.000	0.000	53.067	53.070
ammonium acetate	0.009	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	92.000	92.000	92.000	92.000	108.954	108.953	106.324

	S_33	S_34	S_35	S_36	S_37	S_38
Origin	Storage	CE-100	TA-104	CE-100	DR-100	DR-100
Destination	CE-100	TA-104	SolvRec-102	DR-100	Scrubber-100	Drum-101
Total Mass (kg)	108.954	105.664	662.887	29.608	5.898	23.71
Volume (m^3)	0.141	0.137	0.521	0.021	0.008	0.013
Density (kg/m^3)	773.109	773.689	1272.103	1422.584	773.689	1797.615
Temperature (C)	25	24.352	13.371	24.352	24.352	24.352
Pressure (kPa)	101.325	6.666	101.325	101.325	101.325	101.325
Phase	Liquid	Gaseous	Solid	Solid	Gaseous	Solid
Composition (kg per kg batch)						
acetone-nitrile	0.000	0.000	51.798	0.000	0.000	0.000
methylene chloride	0.000	0.000	343.515	0.000	0.000	0.000
hydroxylamine-hydrochloride	0.000	0.000	0.106	0.000	0.000	0.000
sodium acetate	0.000	0.000	0.000	0.000	0.000	0.000
dichloroacetic acid	0.000	0.000	0.000	0.000	0.000	0.000
carbinol	0.000	0.000	0.232	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000
water	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	1.399	0.000	0.000	0.000
hydroxylamine	0.000	0.000	0.046	0.000	0.000	0.000
hydroxamine	0.000	0.000	0.736	23.686	0.000	23.686
ammonium-dichloroacetate	0.000	0.000	53.071	0.000	0.000	0.000
ammonium acetate	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	108.954	105.664	211.985	5.922	5.898	0.024

Table A.3. Total Stream Table of Stage 3 – N-HYDROXY

	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8	S_9
Origin	Storage	Storage	Storage	Drum-101	ST-101	Storage	Storage	ST-101	ST-100
Destination	ST-100	ST-101	ST-101	ST-101	ST-100	ST-101	ST-101	ST-100	FI-100
Total Mass (kg)	120.500	204.000	13.000	23.000	240.000	37.000	37.000	74.000	434.500
Volume (m^3)	0.116	0.232	0.007	0.013	0.252	0.042	0.036	0.078	0.443
Density (kg/m^3)	1042.013	879.978	1800.000	1800.000	953.047	879.978	1042.013	954.165	981.496
Temperature (C)	25.000	25.000	25.000	25.000	25.000	25.000	25.000	25.000	25.000
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Liquid	Solid	Solid	Liquid	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)									
Tetrahydrofuran	0.000	204.000	0.000	0.000	204.000	37.000	0.000	37.000	241.000
potassium-butoxide	0.000	0.000	13.000	0.000	13.001	0.000	0.000	0.000	2.233
hydroxamine-iv	0.000	0.000	0.000	23.000	22.999	0.000	0.000	0.000	0.230
acetic acid	120.500	0.000	0.000	0.000	0.000	0.000	37.000	37.000	151.736
n-hydroxy	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	22.772
tert-butyl-alcohol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	7.113
Koac	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	9.416

	S_10	S_11	S_12	S_13	S_14	S_15	S_16	S_17	S_18
Origin	FI-100	ST-102	Storage	ST-102	Storage	FI-100	FI-100	ST-102	CN-100
Destination	ST-102	Atm_1	ST-102	Atm_2	FI-100	ST-102	Disposal-100	CN-100	VR-100
Total Mass (kg)	417.857	299.242	241.000	0.024	40.005	42.085	14.562	24.146	24.146
Volume (m^3)	0.431	0.334	0.231	0.000	0.045	0.047	0.010	0.024	0.023
Density (kg/m^3)	969.762	895.053	1042.013	1047.069	879.978	886.295	1488.709	1016.777	1049.009
Temperature (C)	25.000	20.000	25.000	20.000	25.000	25.000	25.000	49.298	20.000
Pressure (kPa)	101.325	7.333	101.325	2.000	101.325	101.325	101.325	7.333	101.325
Phase	Liquid	Gaseous	Liquid	Gaseous	Liquid	Liquid	Solid	Gaseous	Liquid
Composition (kg per kg batch)									
Tetrahydrofuran	237.936	278.092	0.000	0.000	40.005	40.156	2.912	0.000	0.000
potassium-butoxide	0.000	0.000	0.000	0.000	0.000	0.000	2.233	0.000	0.000
hydroxamine-iv	0.230	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
acetic acid	149.810	21.150	241.000	0.024	0.000	1.929	0.000	24.039	24.039
n-hydroxy	22.769	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tert-butyl-alcohol	7.112	0.000	0.000	0.000	0.000	0.000	0.000	0.107	0.107
Koac	0.000	0.000	0.000	0.000	0.000	0.000	9.417	0.000	0.000

	S_19	S_20	S_21	S_22	S_23	S_24	S_25
Origin	VR-100	TA-100	ST-102	CN-100	VR-101	TA-101	ST-102
Destination	TA-100	SolvRec-100	CN-100	VR-101	TA-101	Disposal-101	Drum-100
Total Mass (kg)	24.146	24.146	142.82	142.82	142.82	142.82	234.71
Volume (m^3)	0.023	0.023	0.137	0.136	0.136	0.136	0.213
Density (kg/m^3)	1049.009	1049.009	1042.708	1047.069	1047.069	1047.069	1101.978
Temperature (C)	20	20	24.315	20	20	20	24.315
Pressure (kPa)	101.325	101.325	2	101.325	101.325	101.325	101.325
Phase	Liquid	Liquid	Gaseous	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)							
Tetrahydrofuran	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Potassium-butoxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hydroxamine-iv	0.000	0.000	0.000	0.000	0.000	0.000	0.230
Acetic acid	24.039	24.039	142.820	142.820	142.820	142.820	204.705
n-hydroxy	0.000	0.000	0.000	0.000	0.000	0.000	22.769
tert-butyl-alcohol	0.107	0.107	0.000	0.000	0.000	0.000	7.006
Koac	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table A.4. Total Stream Table for Stage 4 – ACETATE-SALT

	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8
Origin	Storage	Storage	Storage	Storage	Storage	ST-100	Storage	Storage
Destination	ST-100	ST-100	ST-100	ST-100	ST-100	Atm-100	ST-100	TA-100
Total Mass (kg)	164.129	140.226	4.700	110.759	4509.560	3941.786	181.758	0.200
Volume (m^3)	0.141	0.141	0.003	0.141	0.000	0.387	0.000	0.000
Density (kg/m^3)	1164.621	995.011	1800.000	785.923	0.000	10196.734	0.000	0.000
Temperature (C)	25.000	25.000	25.000	25.000	25.000	25.000	25.000	25.000
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	377.143	101.325
Phase	Liquid	Liquid	Solid	Liquid	Gaseous	Gaseous	Gaseous	Gaseous
Composition (kg per kg batch)								
acetic acid	123.097	0.000	0.000	0.000	0.000	109.109	0.000	0.000
n-hydroxy	32.826	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tert-butyl-alcohol	8.206	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	0.000	140.226	0.000	0.000	0.000	140.209	0.000	0.000
palladium-catalyst	0.000	0.000	4.700	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	0.000	0.000	110.759	0.000	110.764	0.000	0.000
nitrogen	0.000	0.000	0.000	0.000	4509.560	3581.704	0.000	0.000
hydrogen	0.000	0.000	0.000	0.000	0.000	0.000	181.758	0.200
hypo9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
mk-vi-acetate-salt	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
toluene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
isopropyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbon	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
super-cel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_9	S_10	S_11	S_12	S_13	S_14	S_15	S_16
Origin	TA-100	ST-100	ST-100	FI-100	Storage	Storage	FI-100	FI-100
Destination	ST-100	Scrubber-100	FI-100	ST-101	FI-100	FI-100	ST-101	SolvRec-100
Total Mass (kg)	0.200	1093.979	73.538	65.559	20.400	5.000	27.504	5.875
Volume (m^3)	0.000	0.000	0.036	0.028	0.022	0.003	0.028	0.004
Density (kg/m^3)	0.000	0.000	2065.533	2355.513	940.029	1800.000	968.845	1521.598
Temperature (C)	25.000	25.000	25.000	25.000	25.000	25.000	25.000	25.000
Pressure (kPa)	101.325	101.325	5.295	101.325	101.325	101.325	101.325	101.325
Phase	Gaseous	Gaseous	Solid	Solid	Liquid	Solid	Liquid	Solid
Composition (kg per kg batch)								
acetic acid	0.000	0.000	5.840	0.000	7.598	0.000	13.001	0.438
n-hydroxy	0.000	0.000	0.657	0.656	0.000	0.000	0.000	0.000
tert-butyl-alcohol	0.000	0.000	8.207	8.207	0.000	0.000	0.000	0.000
water	0.000	0.000	2.320	0.000	7.028	0.000	8.944	0.405
palladium-catalyst	0.000	0.000	4.700	0.000	0.000	0.000	0.000	4.700
ethanol	0.000	0.000	0.000	0.000	5.773	0.000	5.441	0.333
nitrogen	0.000	914.851	13.028	12.930	0.000	0.000	0.099	0.000
hydrogen	0.200	179.128	2.551	2.532	0.000	0.000	0.019	0.000
hypo9	0.000	0.000	0.000	5.000	0.000	5.000	0.000	0.000
mk-vi-acetate-salt	0.000	0.000	36.234	36.234	0.000	0.000	0.000	0.000
toluene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
isopropyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

carbon	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
super-cel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_17	S_18	S_19	S_20	S_21	S_22	S_23	S_24
Origin	ST-101	ST-101	CN-100	VR-100	TA-101	Storage	ST-101	CN-100
Destination	Atm_1	CN-100	VR-100	TA-101	Disposal-100	ST-101	CN-100	VR-101
Total Mass (kg)	14.563	28.122	28.122	28.122	28.122	278.190	140.383	140.383
Volume (m^3)	0.000	0.029	0.028	0.028	0.028	0.280	0.142	0.141
Density (kg/m^3)	1558065.980	984.354	1004.368	1004.368	1004.368	995.011	991.570	996.338
Temperature (C)	20.000	44.981	20.000	20.000	20.000	25.000	38.091	20.000
Pressure (kPa)	6.666	6.666	101.325	101.325	101.325	101.325	6.666	101.325
Phase	Gaseous	Gaseous	Liquid	Liquid	Liquid	Liquid	Gaseous	Liquid
Composition (kg per kg batch)								
acetic acid	0.002	12.738	12.738	12.738	12.738	0.000	0.094	0.094
n-hydroxy	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tert-butyl-alcohol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	0.002	8.922	8.922	8.922	8.922	278.190	140.289	140.289
palladium-catalyst	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethanol	0.004	5.437	5.437	5.437	5.437	0.000	0.000	0.000
nitrogen	12.171	0.857	0.857	0.857	0.857	0.000	0.000	0.000
hydrogen	2.383	0.168	0.168	0.168	0.168	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
mk-vi-acetate-salt	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
toluene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
isopropyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbon	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
super-cel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_25	S_26	S_27	S_28	S_29	S_30	S_31	S_32
Origin	VR-101	TA-102	ST-101	Storage	Storage	ST-101	EX-100	EX-100
Destination	TA-102	Disposal-101	Atm-101	ST-101	ST-101	EX-100	ST-102	TA-103
Total Mass (kg)	140.383	140.383	137.920	140.226	20.200	210.691	189.112	21.579
Volume (m^3)	0.141	0.141	0.139	0.141	0.023	0.192	0.168	0.024
Density (kg/m^3)	996.338	996.338	995.011	995.011	864.607	1095.723	1124.659	894.117
Temperature (C)	20.000	20.000	25.000	25.000	25.000	25.000	25.000	25.000
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Liquid	Gaseous	Liquid	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)								
acetic acid	0.094	0.094	0.000	0.000	0.000	0.169	0.168	0.000
n-hydroxy	0.000	0.000	0.000	0.000	0.000	0.657	0.000	0.656
tert-butyl-alcohol	0.000	0.000	0.000	0.000	0.000	8.206	8.207	0.000
water	140.289	140.289	137.920	140.226	0.000	140.225	140.211	0.014
palladium-catalyst	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
nitrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hydrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	0.000	0.000	5.000	5.000	0.000
mk-vi-acetate-salt	0.000	0.000	0.000	0.000	0.000	36.235	35.523	0.710
toluene	0.000	0.000	0.000	0.000	20.200	20.199	0.002	20.198
isopropyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbon	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

super-cel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_33	S_34	S_35	S_36	S_37	S_38	S_39	S_40
Origin	TA-103	Storage	Storage	ST-102	EX-101	Storage	EX-100	TA-104
Destination	SolvRec-101	ST-102	ST-102	EX-101	EX-100	EX-100	TA-104	Disposal-102
Total Mass (kg)	21.579	150.300	41.900	381.312	195.838	50.800	195.463	195.463
Volume (m^3)	0.024	0.173	0.044	0.382	0.192	0.058	0.192	0.192
Density (kg/m^3)	894.117	868.630	947.574	998.186	1018.763	868.630	1017.647	1017.647
Temperature (C)	25.000	25.000	25.000	12.153	12.153	25.000	13.620	13.620
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)								
acetic acid	0.000	0.000	0.000	0.168	0.168	0.000	0.168	0.168
n-hydroxy	0.656	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tert-butyl-alcohol	0.000	0.000	0.000	8.206	8.208	0.000	8.207	8.207
water	0.014	0.000	31.195	171.407	171.390	0.000	171.372	171.372
palladium-catalyst	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
nitrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hydrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	4.999	5.000	0.000	5.000	5.000
mk-vi-acetate-salt	0.710	0.000	0.000	35.523	0.353	0.000	0.004	0.004
toluene	20.198	0.000	0.000	0.004	0.002	0.000	0.002	0.002
isopropyl acetate	0.000	150.300	0.000	150.302	0.016	50.800	0.006	0.006
ammonium hydroxide	0.000	0.000	10.705	10.703	10.705	0.000	10.706	10.706
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbon	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
super-cel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_41	S_42	S_43	S_44	S_45	S_46	S_47	S_48
Origin	EX-100	Storage	EX-101	EX-101	Storage	Storage	ST-103	FI-101
Destination	EX-101	EX-101	TA-105	ST-103	ST-103	ST-103	FI-101	ST-104
Total Mass (kg)	51.175	69.700	69.926	236.423	2.300	2.000	240.723	234.580
Volume (m^3)	0.058	0.056	0.057	0.249	0.001	0.001	0.251	0.247
Density (kg/m^3)	884.395	1234.791	1235.863	950.716	2250.021	1800.000	959.648	947.999
Temperature (C)	13.620	25.000	16.986	16.986	25.000	25.000	17.100	20.000
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Liquid	Liquid	Liquid	Solid	Solid	Liquid	Liquid
Composition (kg per kg batch)								
acetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
n-hydroxy	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tert-butyl-alcohol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	0.017	44.608	44.597	0.045	0.000	0.000	0.046	0.045
palladium-catalyst	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
nitrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hydrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
mk-vi-acetate-salt	0.348	0.000	0.036	35.485	0.000	0.000	35.485	35.485
toluene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
isopropyl acetate	50.810	0.000	0.201	200.893	0.000	0.000	200.893	199.051
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	25.092	25.092	0.000	0.000	0.000	0.000	0.000

carbon	0.000	0.000	0.000	0.000	2.300	0.000	2.299	0.000
super-cel	0.000	0.000	0.000	0.000	0.000	2.000	2.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_49	S_50	S_51	S_52	S_53	S_54	S_55	S_56
Origin	Storage	FI-101	FI-101	ST-104	ST-104	CN-100	VR-102	ST-104
Destination	FI-101	ST-104	Disposal-104	Atm_2	CN-100	VR-102	SolvRec-102	ATM-102
Total Mass (kg)	25.400	26.168	5.375	220.945	0.896	0.896	0.896	3.396
Volume (m^3)	0.029	0.030	0.003	0.253	0.001	0.001	0.001	0.004
Density (kg/m^3)	868.630	869.996	1595.446	874.230	896.227	896.331	896.331	868.630
Temperature (C)	25.000	23.784	23.784	20.000	0.096	0.000	0.000	25.000
Pressure (kPa)	101.325	101.325	101.325	2.000	2.000	101.325	101.325	101.325
Phase	Liquid	Liquid	Solid	Gaseous	Gaseous	Liquid	Liquid	Gaseous
Composition (kg per kg batch)								
acetic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
n-hydroxy	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tert-butyl-alcohol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	0.000	0.001	0.000	0.015	0.002	0.002	0.002	0.000
palladium-catalyst	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
nitrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hydrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
mk-vi-acetate-salt	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
toluene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
isopropyl acetate	25.400	26.167	1.075	220.930	0.894	0.894	0.894	3.396
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbon	0.000	0.000	2.300	0.000	0.000	0.000	0.000	0.000
super-cel	0.000	0.000	2.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_57	S_58	S_59	S_60	S_61	S_62	S_63	S_64
Origin	Storage	Storage	ST-104	CE-100	Storage	CE-100	TA-106	CE-100
Destination	ST-104	ST-104	CE-100	TA-106	CE-100	TA-106	SolvRec-103	DR-100
Total Mass (kg)	230.300	7.300	273.111	234.472	38.500	33.670	268.142	43.469
Volume (m^3)	0.298	0.007	0.318	0.294	0.050	0.043	0.338	0.031
Density (kg/m^3)	773.109	1042.013	857.859	797.169	773.109	774.995	794.344	1423.464
Temperature (C)	25.000	25.000	10.000	10.000	25.000	22.895	11.672	22.895
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Solid
Composition (kg per kg batch)								
acetic acid	0.000	7.300	7.300	7.299	0.000	0.000	7.299	0.000
n-hydroxy	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
tert-butyl-alcohol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
water	0.000	0.000	0.027	0.026	0.000	0.000	0.027	0.000
palladium-catalyst	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
nitrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hydrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
hypo9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
mk-vi-acetate-salt	0.000	0.000	35.485	0.710	0.000	0.000	0.711	34.775
toluene	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
isopropyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

sodium chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
carbon	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
super-cel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
cyclohexane	230.300	0.000	230.301	226.437	38.500	33.670	260.106	8.694

	S_65	**S_66**
Origin	DR-100	DR-100
Destination	Scrubber-101	Drum-100
Total Mass (kg)	8.589	34.880
Volume (m^3)	0.011	0.019
Density (kg/m^3)	773.109	1792.856
Temperature (C)	25.000	25.000
Pressure (kPa)	101.325	101.325
Phase	Gaseous	Solid
Composition (kg per kg batch)		
acetic acid	0.000	0.000
n-hydroxy	0.000	0.000
tert-butyl-alcohol	0.000	0.000
water	0.000	0.000
palladium-catalyst	0.000	0.000
ethanol	0.000	0.000
nitrogen	0.000	0.000
hydrogen	0.000	0.000
hypo9	0.000	0.000
mk-vi-acetate-salt	0.000	34.775
toluene	0.000	0.000
isopropyl acetate	0.000	0.000
ammonium hydroxide	0.000	0.000
sodium chloride	0.000	0.000
carbon	0.000	0.000
super-cel	0.000	0.000
cyclohexane	8.589	0.105

Table A.5. Total Stream Table for Stage 6 – MK-MALEATE

	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8
Origin	Storage	Storage	Drum-100	Storage	ST-100	EX-100	EX-100	TA-100
Destination	ST-100	ST-100	ST-100	ST-100	EX-100	ST-101	TA-100	Disposal-100
Total Mass (kg)	144.800	67.851	10.900	14.800	238.351	159.307	79.044	79.044
Volume (m^3)	0.080	0.068	0.006	0.016	0.170	0.091	0.079	0.079
Density (kg/m^3)	1800.000	995.011	1800.000	947.574	1399.512	1750.945	996.435	996.435
Temperature (C)	25.000	25.000	25.000	25.000	25.000	25.000	25.000	25.000
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Solid	Liquid	Solid	Liquid	Solid	Solid	Liquid	Liquid
Composition (kg per kg batch)								
methylene-chloride	144.800	0.000	0.000	0.000	144.801	144.656	0.145	0.145
Water	0.000	67.851	0.000	11.019	78.870	0.078	78.791	78.791
l-malate-salt-vii	0.000	0.000	10.900	0.000	10.900	10.791	0.108	0.108
ammonium hydroxide	0.000	0.000	0.000	3.781	3.780	3.782	0.000	0.000
Ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Nitrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
maleic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
maleate-viii	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

malic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_9	S_10	S_11	S_12	S_13	S_14	S_15	S_16
Origin	ST-101	ST-101	CN-100	VR-100	TA-101	Storage	ST-101	CN-100
Destination	Atm_1	CN-100	VR-100	TA-101	SolvRec-100	ST-101	CN-100	VR-101
Total Mass (kg)	3.649	38.915	38.915	38.915	38.915	37.6	10.882	10.882
Volume (m^3)	0	0.039	0.022	0.022	0.022	0.048	0.014	0.014
Density (kg/m^3)	4381080.734	1000.851	1797.486	1797.486	1797.486	785.923	794.472	790.831
Temperature (C)	20	39.863	20	20	20	25	23.709	20
Pressure (kPa)	7.333	7.333	101.325	101.325	101.325	101.325	7.333	101.325
Phase	Gaseous	Gaseous	Solid	Solid	Solid	Liquid	Gaseous	Liquid
Composition (kg per kg batch)								
methylene-chloride	0.000	36.164	36.164	36.164	36.164	0.000	0.000	0.000
Water	0.001	0.019	0.019	0.019	0.019	0.000	0.007	0.007
l-malate-salt-vii	0.000	2.698	2.698	2.698	2.698	0.000	0.000	0.000
ammonium hydroxide	3.648	0.033	0.033	0.033	0.033	0.000	0.100	0.100
Ethanol	0.000	0.000	0.000	0.000	0.000	37.600	10.775	10.775
Nitrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
maleic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
maleate-viii	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
malic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_17	S_18	S_19	S_20	S_21	S_22	S_23	S_24
Origin	Storage	VR-101	TA-102	ST-101	Storage	Storage	TA-103	Storage
Destination	ST-101	TA-102	SolvRec-101	ST-102	TA-103	ST-102	ST-102	ST-102
Total Mass (kg)	209.089	10.882	10.882	352.552	11.2	2.3	11.2	4.401
Volume (m^3)	0	0.014	0.014	0.099	0.011	0.001	0.011	0.006
Density (kg/m^3)	0	790.831	790.831	3563.338	1051.894	1800	1051.894	785.923
Temperature (C)	25	20	20	24.616	25	25	25	25
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Gaseous	Liquid	Liquid	Gaseous	Liquid	Solid	Liquid	Liquid
Composition (kg per kg batch)								
methylene-chloride	0.000	0.000	0.000	108.491	0.000	0.000	0.000	0.000
water	0.000	0.007	0.007	0.049	0.000	0.000	0.000	0.000
l-malate-salt-vii	0.000	0.000	0.000	8.095	0.000	0.000	0.000	0.000
ammonium hydroxide	0.000	0.100	0.100	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	10.775	10.775	26.826	5.600	0.000	5.600	4.401
nitrogen	209.089	0.000	0.000	209.088	0.000	0.000	0.000	0.000
maleic acid	0.000	0.000	0.000	0.000	5.600	0.000	5.600	0.000
maleate-viii	0.000	0.000	0.000	0.000	0.000	2.300	0.000	0.000
malic acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethyl acetate	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	S_25	S_26	S_27	S_28	S_29	S_30	S_31	S_32
Origin	Storage	ST-102	CE-100	Storage	CE-100	Storage	Storage	CE-100
Destination	ST-102	CE-100	TA-104	CE-100	TA-104	ST-102	CE-100	TA-104
Total Mass (kg)	23.7	394.153	381.761	16.1	17.649	16.1	16.1	14.551
Volume (m^3)	0.027	0.142	0.133	0.019	0.021	0.019	0.019	0.017
Density (kg/m^3)	893.628	2780.202	2879.995	832.674	835.324	832.674	832.674	833.29
Temperature (C)	25	3	3	25	20.602	25	25	24.391
Pressure (kPa)	101.325	101.325	101.325	101.325	101.325	101.325	101.325	101.325
Phase	Liquid	Gaseous	Gaseous	Liquid	Liquid	Liquid	Liquid	Liquid
Composition (kg per kg batch)								
methylene-chloride	0.000	108.491	108.493	0.000	0.000	0.000	0.000	0.000
water	0.000	0.051	0.050	0.000	0.003	0.000	0.000	0.000
l-malate-salt-vii	0.000	0.406	0.405	0.000	0.000	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ethanol	0.000	37.709	35.427	8.600	9.722	8.600	8.600	7.773
nitrogen	0.000	209.090	209.090	0.000	0.000	0.000	0.000	0.000
maleic acid	0.000	3.378	3.379	0.000	0.000	0.000	0.000	0.000
maleate-viii	0.000	8.762	0.088	0.000	0.000	0.000	0.000	0.000
malic acid	0.000	2.570	2.569	0.000	0.000	0.000	0.000	0.000
ethyl acetate	23.700	23.700	22.268	7.500	7.923	7.500	7.500	6.778

	S_33	S_34	S_35	S_36
7Origin	TA-104	CE-100	DR-100	DR-100
Destination	SolvRec-102	DR-100	Scrubber-100	Drum-101
Total Mass (kg)	413.961	12.392	3.709	8.683
Volume (m^3)	0.171	0.009	0.004	0.005
Density (kg/m^3)	2425.709	1335.278	832.674	1797.911
Temperature (C)	6.08	24.391	25	25
Pressure (kPa)	101.325	101.325	101.325	101.325
Phase	Gaseous	Solid	Gaseous	Solid
Composition (kg per kg batch)				
methylene-chloride	108.491	0.000	0.000	0.000
water	0.050	0.000	0.000	0.000
l-malate-salt-vii	0.406	0.000	0.000	0.000
ammonium hydroxide	0.000	0.000	0.000	0.000
ethanol	52.925	1.986	1.981	0.005
nitrogen	209.088	0.000	0.000	0.000
maleic acid	3.378	0.000	0.000	0.000
maleate-viii	0.087	8.674	0.000	8.674
malic acid	2.567	0.000	0.000	0.000
ethyl acetate	36.967	1.732	1.728	0.004

Figure A.1. Example of Batch Design Kit Display