Production of Polysilicon using a Modified Siemens Process

ENES489P: Hands-On Systems Engineering Project Report

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May 11, 2011

Project Abstract

Systems engineering is a unique approach to modeling many different processes. A high level approach is used to analyze the design of an alternative version of a polysilicon production facility. The system functions by structuring the pathways of the chemical process. The Siemens process is currently the de facto standard in the production of polysilicon. This system strives to improve upon this design as well as to create additional profit through an additional process reaction that utilizes the waste products of the Siemens product. The primary flow of the entire process is to first convert metallurgical grade silicon to a chlorosilane intermediate which then deposits to form the desired polysilicon product but also forms a tetrachlorosilane as a waste byproduct. The additional process converts the tetrachlorosilane to silicon dioxide which can be further processed by the silicone industry.

The structure of the process include the primary manufacturing equipment and specifically the deposition reactor. Different operating parameters for the deposition reactors are considered in order to optimize the performance, cost, and safety of the reactor. These factors are subjected to a trade-off analysis to determine the optimal combinations of components and further used in the system entirety to meet the goal of a minimum 10% return on investment.

Contents

Project Description

Problem Statement

The majority of companies utilize the Siemens process for the production of solar grade polysilicon. For every one mole of Si converted to polysilicon, three to four moles are converted to tetrachlorosilane (TET), a toxic byproduct that is produced during the production of polysilicon. This is a significant quantity of waste. Unfortunately, A popular solution has been to dump TET in waste disposal sites. To avoid this chemical dumping, an alternative hydrolysis reaction is being added on to the polysilicon production system to produce silicon dioxide, a neutral compound that is further used in the production of silicone and evaluated as system.

Customer Requirements

The investors require a 10% return on investment and a nearly complete elimination of TET exiting the process.

Objectives

The purpose of this report is to demonstrate the implementation and functionality to which high level systems concepts can be used to think about current chemical process design. This study lays out a new framework to approach the design of polysilicon production as well as tackle a pressing environmental waste issue. To provide a detailed analysis of the system designed, the following issues will be addressed:

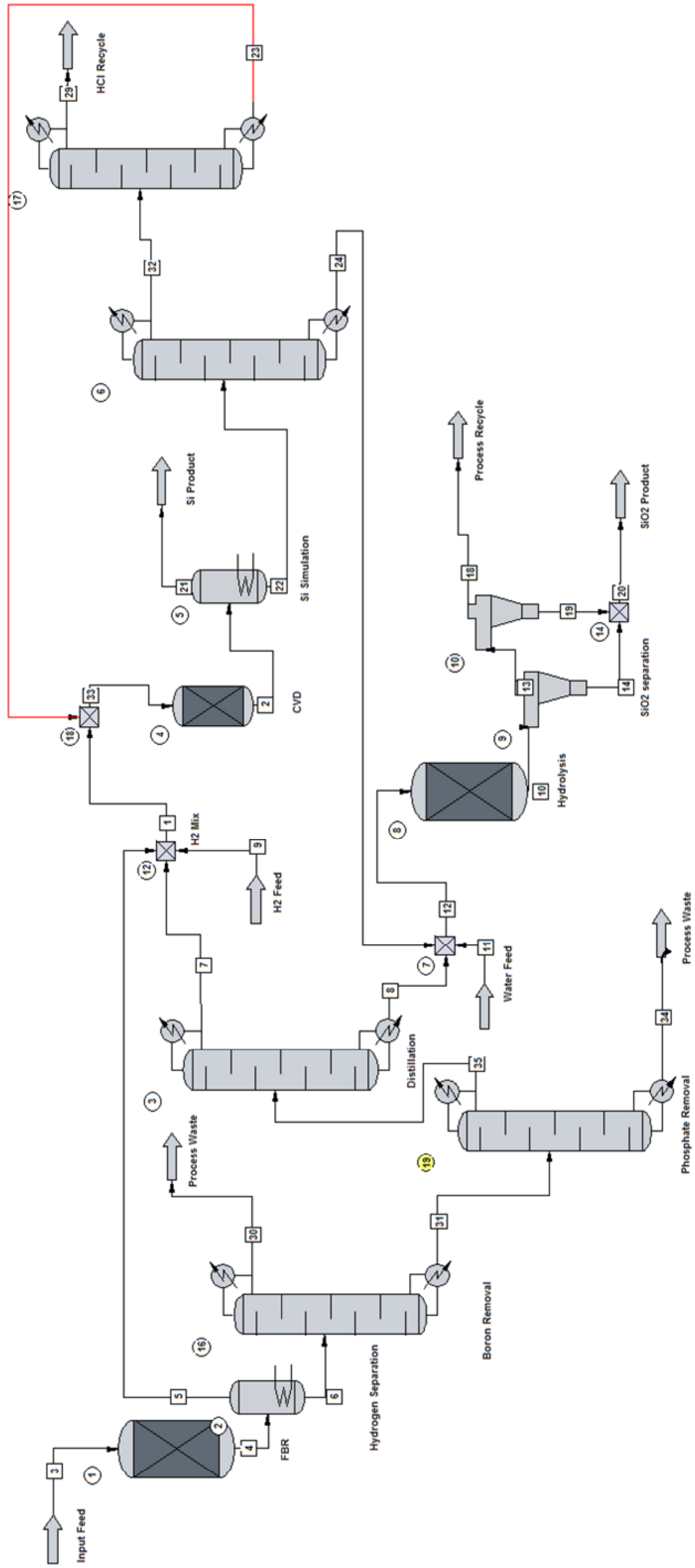
1. How will the system go about producing products?
2. What are the system requirements?
3. What should the system produce?
4. What should objects be classified as?
5. How will objects and actors interact?
6. How will the investment be justified?

Terminology

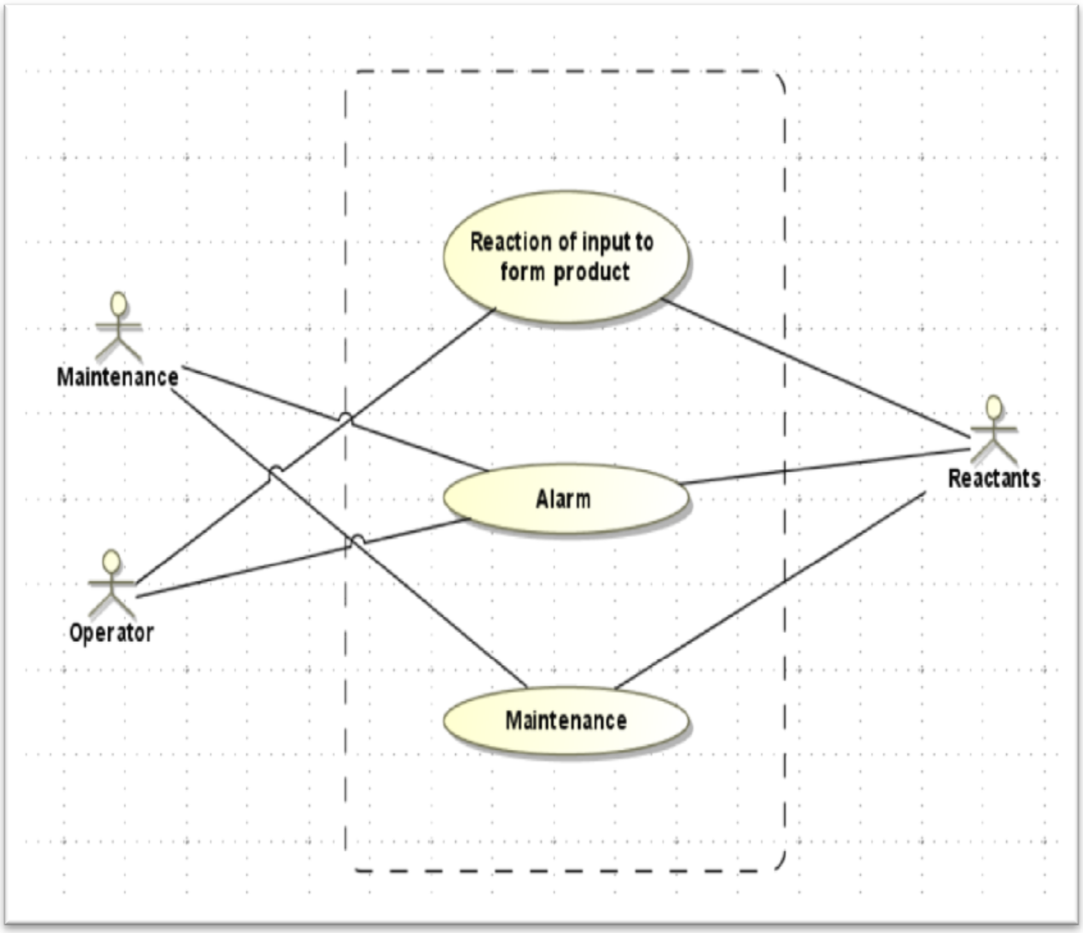
- Distillation Column: A tall metal cylinder internally fitted with perforated horizontal plates used to promote separation of miscible liquids.
- Fluidized Bed Reactor: a type of reactor device that can be used to carry out a variety of multiphase chemical reactions.
- Chemical Vapor Deposition: a chemical process used to produce high-purity, high-performance solid materials.
- Polysilicon: 99.9999% pure silicon

System Structure

ChemCAD Process Flow Diagram

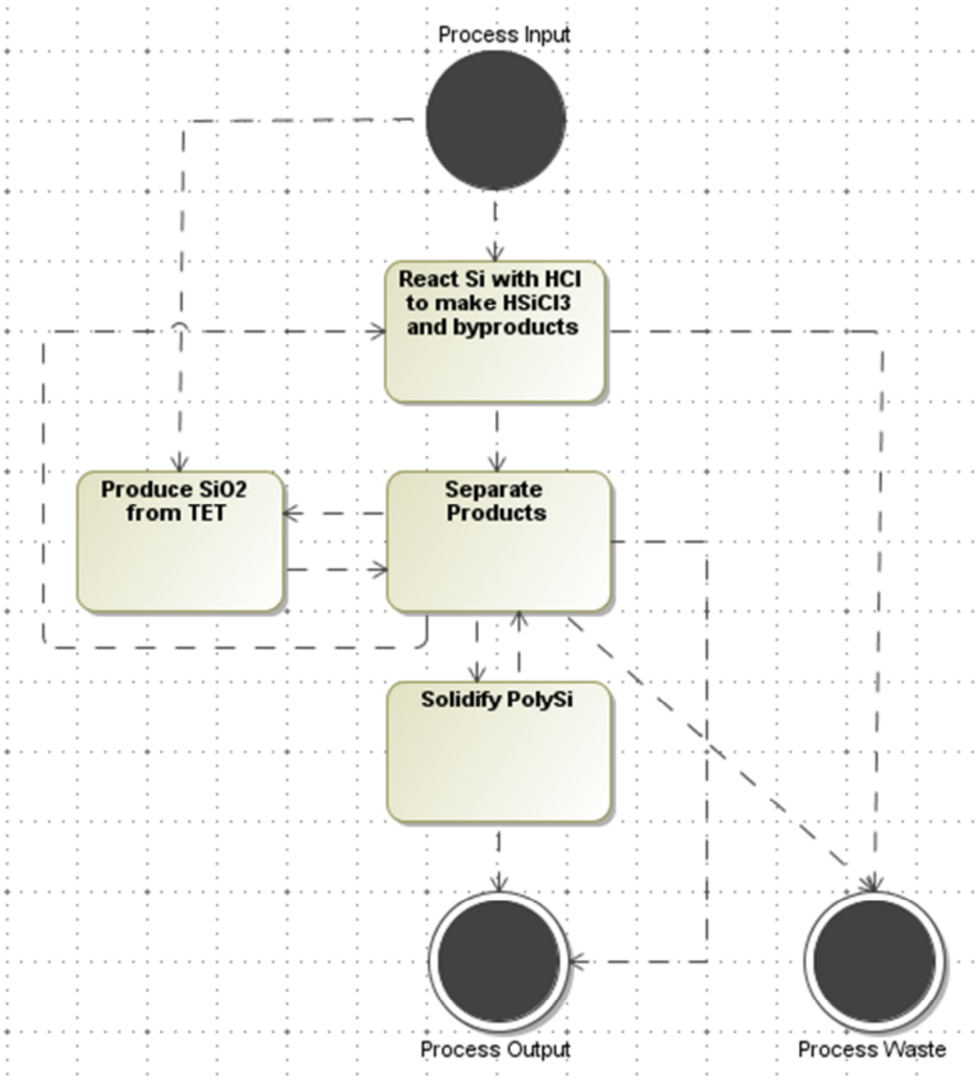


Use Case Diagram

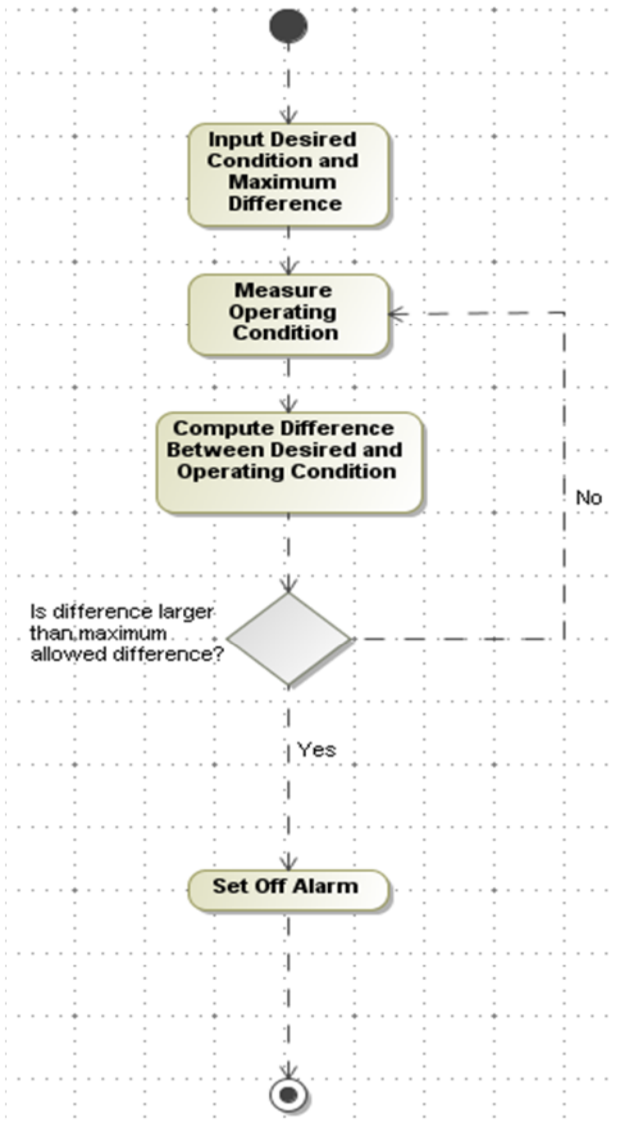


Activity Diagrams

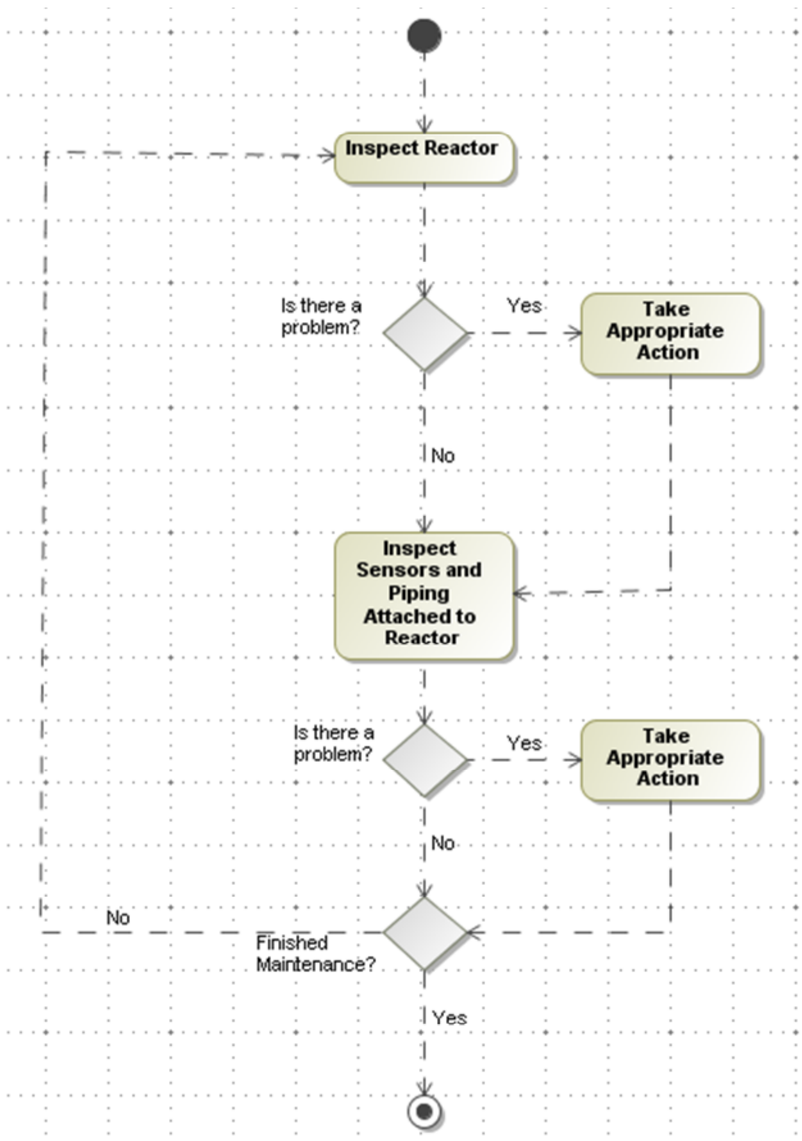
Use Case 1



Use Case 2


Input Desired Condition and Maximum Difference
Measure Operating Condition
Compute Difference Between Desired and Operating Condition
No
Is difference larger than maximum allowed difference?
Yes
Set Off Alarm

Use Case 3



Textual Scenarios

Use Case 1: Reaction from Input to form Product

The first use case addresses the primary function of the system, which is to produce polysilicon product from an input of metallurgical grade silicon (MG-Si) and hydrogen chloride (HCl). This use case also addresses the goal of dealing with the toxic tetrachlorosilane by forming it into another product, namely silicon dioxide $(SiO)_2$. Although the specific conditions of the process may be variable, the generalized behavior of the system is as follows: MG-Si is fed in with HCl to form trichlorosilane (TCS) and impurities. The TCS is then isolated and reactor to form polysilicon rods. The TET byproducts are then reacted with water in a separate reactor to for SiO_2. The individual scenarios detail the individual reactions and subsystems that together comprise the overall process:

Scenario (1.1): Formation of chlorosilanes

Description: MG-Si is reacted with dry HCl to form TCS, TET, and other impurities

Primary Object: Fluidized Bed Reactor

Primary Actors: Solid Si and HCl

Pre-condition: FBR is at specified operating conditions

Flow of Events:

1. Solid Si is fed into the reactor
2. HCl is inputted through bottom of system
3. HCl reacts with Si to form silicon chlorides
4. Vapor collected from top of reactor
5. Unreacted mass removed through bottom of reactor

Post-condition: Trichlorosilane is produced, along with tetracholorsilane, hydrogen(H_2), boron trichloride (BCl_3), and Phosphate Pentachloride (PCl_5).

Scenario (1.2): Separation of FBR products

Description: Products from the FBR are separated into desirables and undesirables via a series of distillation columns

Primary Object: Distillation Column

Primary Actors: H_2, TCS,TET, BCl_3, PCl_5

Pre-condition: FBR products are fed in at proper conditions and distillation column is maintained at proper conditions

Flow of Events:

1. FBR products are fed into column
2. FBR products undergo reflux
3. Low boiling impurities exit at the top of the column

4. High boiling impurities exit at the bottom of the column

Post-condition: The desired compound is isolated at a certain purity level and passed onto the next step in the reaction

Scenario (1.2.1): Separation of H_2

Description: H_2 is removed from the FBR products

Primary Object: Flash Distillation Drum

Primary Actors: H_2, TCS,TET, BCl_3, P_2Cl_5

Pre-condition: Inputs are fed in at proper conditions and the distillation drum is maintained at proper conditions

Flow of Events:

1. FBR products are fed into drum
2. Products cooled until only H_2 remains as gas
3. H_2 exits and other compounds are isolated

Post-condition: All H_2 is removed from the FBR product stream. The H_2-free stream continues through the rest of the process. The removed H_2 is recycled for use later in the process.

Scenario (1.2.2): Separation of BCl_3

Description: BCl_3 is removed from the H_2 separation products

Primary Object: Distillation Column

Primary Actors: TCS,TET, BCl_3, P_2Cl_5

Pre-condition: Inputs are fed in at proper conditions and the distillation column is maintained at proper conditions

Flow of Events:

4. H_2 separation products are fed into column
5. H_2 separation column products undergo reflux
6. BCl_3 boils most easily and exits at the top of the column, with a small amount of other compounds
7. Other compounds exit at the bottom of the column

Post-condition: All BCl_3 is removed from the H_2 separations product stream and exits the process as waste. The BCl_3-free stream continues through the rest of the process.

Scenario (1.2.3): Separation of PCl_5

Description: PCl_5 is removed from the BCl_3 separation products

Primary Object: Distillation Column

Primary Actors: TCS,TET, P_2Cl_5

Pre-condition: Inputs are fed in at proper conditions and distillation column is maintained at proper conditions

Flow of Events:

1. BCl_3 separation products are fed into column
2. BCl_3 separation products undergo reflux
3. PCl_5 boils least readily and is separated from the other compounds and exits at the bottom of the column
4. All other compounds exit at the top of the column

Post-condition: All PCl_5 is removed from the BCl_3 separations product stream and exits the process as waste. The PCl_5-free stream continues through the rest of the process.

Scenario (1.2.4): Separation of TET

Description: TET is removed from the PCl_5 products

Primary Object: Distillation Column

Primary Actors: TCS,TET

Pre-condition: Inputs are fed in at proper conditions and distillation column is maintained at proper conditions

Flow of Events:

1. PCl_5 separation products are fed into column
2. PCl_5 separation products undergo reflux
3. TET boils less readily and is separated from TCS and exits at the bottom of the column
4. TCS exits at the top of the column

Post-condition: Most TET is removed from the TCS product stream at the top of the column. Both streams go on to be processed further

Scenario (1.3): Formation of polysilicon

Description: TCS is reacted with H_2 to form polysilicon rods

Primary Object: Siemens CVD reactor

Primary Actors: TCS, H_2

Pre-condition: CVD is at specified operating conditions, silicon will only deposit on the seed rods

Flow of Events:

1. TCS is mixed with H_2 and fed into the CVD reactor
2. TCS reacts with $H_2$to form TET, HCl, and the desired polysilicon
3. Polysilicon deposits onto the silicon seed rods of the CVD reactor
4. Other compounds pass through the CVD for further processing
5. Polysilicon rods collected at the end of the process

Post-condition: Polysilicon rods of 99.9999% purity are formed.

Scenario (1.4): Separation of CVD products

Description: Products from the CVD are separated into desirables and undesirables via a series of distillation columns

Primary Object: Distillation Column

Primary Actors: TCS,TET, HCl, DCS

Pre-condition: CVD products are fed in at proper conditions and distillation column is maintained at proper conditions

Flow of Events:

1. CVD products are fed into column
2. CVD products undergo reflux
3. Low boiling impurities exit at the top of the column
4. High boiling impurities exit at the bottom of the column

Post-condition: The desired compound is isolated at a certain purity level and passed onto the next step in the reaction

Scenario (1.4.1): Separation of TET

Description: TET is removed from the CVD products

Primary Object: Distillation Column

Primary Actors: TCS,TET, HCl, DCS

Pre-condition: Inputs are fed in at proper conditions and distillation column is maintained at proper conditions

Flow of Events:

1. CVD products are fed into column
2. CVD products undergo reflux
3. TET boils least readily and is separated from TCS and exits at the bottom of the column
4. TCS, HCl, and DCS exits at the top of the column

Post-condition: Most TET is removed from stream at the top of the column. Both streams go on to be processed further

Scenario (1.4.2): Separation of HCl

Description: HCl is removed from the CVD products for recycle

Primary Object: Distillation Column

Primary Actors: TCS, HCl, DCS

Pre-condition: Inputs are fed in at proper conditions and distillation column is maintained at proper conditions

Flow of Events:

1. TET Separation products are fed into column
2. TET Separation products undergo reflux
3. HCl boils most easily and exits at the top of the column
4. TCS, DCS exit at bottom

Post-condition: Most HCl is removed from stream at the bottom of the column. Both streams are recycled back into the process

Scenario (1.5): Formation of SiO_2

Description: TET is reacted with H_2O to form SiO_2

Primary Object: Hydrolysis Reactor

Primary Actors: TET, H_2O

Pre-condition: TET from other parts in the process is mixed with water and fed in at the proper conditions

Flow of Events:

1. TET and H_2O are mixed and enter the reactor
2. TET reacts with H_2O to form SiO_2 and HCl
3. Products exit the reactor

Post-condition: SiO_2 is formed and most of the TET formed from the earlier stages in the process is consumed

Scenario (1.5.1): Separation of SiO_2

Description: Solid SiO_2 products are separated from the other compounds

Primary Object: Cyclone

Primary Actors: SiO_2, HCl

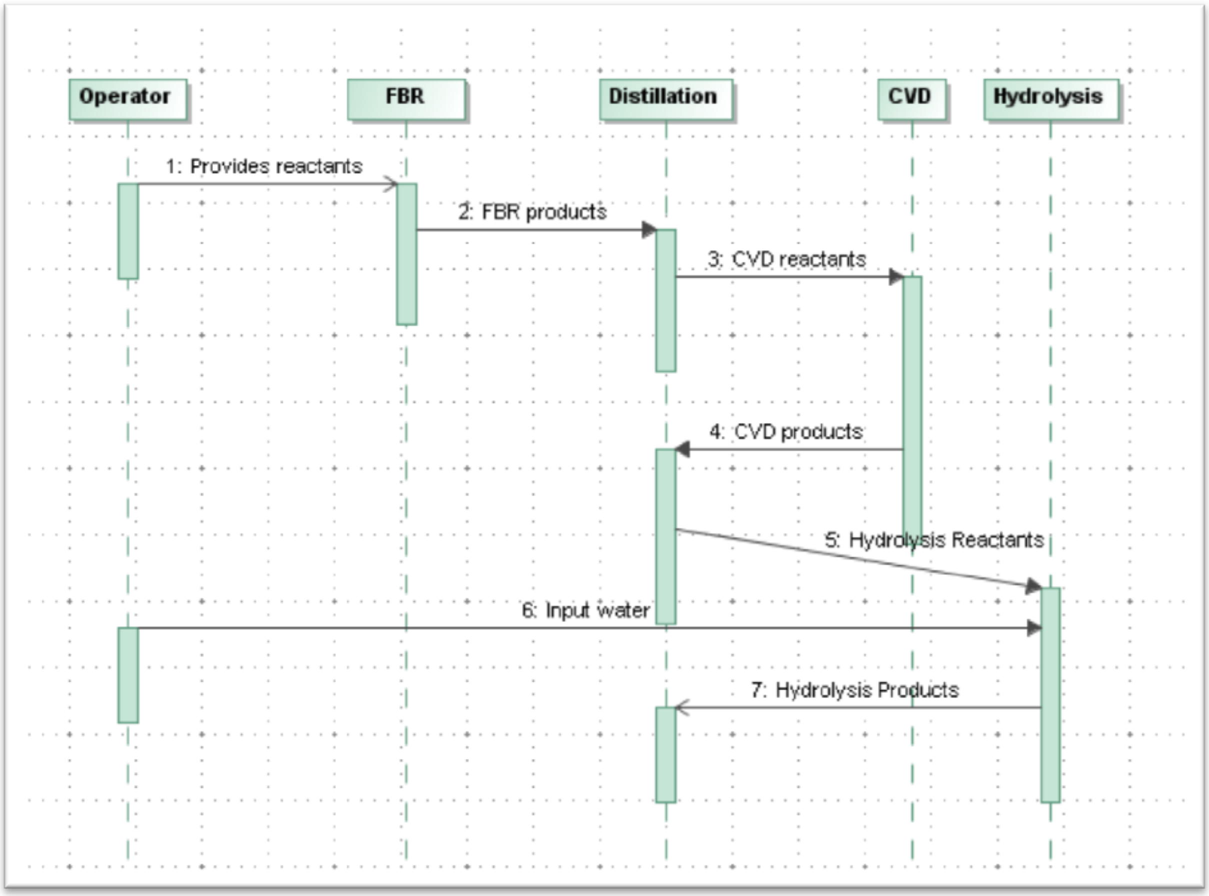
Pre-condition: Inputs are fed in at proper conditions and cyclone is maintained at proper conditions. SiO_2 is a solid.

Flow of Events:

1. SiO_2, HCl product and small amounts of TCS, TET, and water are fed into the cyclone
2. Solid SiO_2 falls to the bottom and exits the cyclone
3. Gaseous compounds exit through the top of the cyclone

Post-condition: All SiO_2 is separated from the hydrolysis reactor product stream.

<u>Sequence Diagram for Use Case 1</u>



Use Case 2: Alarm

The second use case addresses the necessity of preventing accidents and dangerous operating conditions within the plant. Sensors must be used throughout the system to monitor the temperature, pressure, and flow rates. Should any of these conditions fall outside of normal or allowable operating conditions, the system must trigger an alarm to notify the operators of the issue.

Scenario (2.1): Temperature sensors

Description: Temperature sensors detect the difference between the desired operating temperature and the actual operating temperature and alerts if there is a certain difference between the two.

Primary Object: Temperature sensor

Primary Actors: Streams of reactants and products throughout the system

Pre-condition: Desired operating temperature and maximum allowable difference are specified

Flow of Events:

1. Temperature sensor takes reading of the operating temperature
2. Sensor compares operating temperature to desired temperature
3. Sensor compares the difference in the actual and desired temperature to the specified allowable difference
4. If the difference is smaller, then alarm does nothing. If it is larger, the alarm goes off.

Post-condition: The appropriate action is taken based on the operating temperature. If there is a dangerous condition, the alarm goes off, if not, then process goes on as normal.

Scenario (2.2): Pressure

Description: Pressure sensors detect the difference between the desired operating pressure and the actual operating pressure and alerts if there is a certain difference between the two.

Primary Object: Pressure sensor

Primary Actors: Streams of reactants and products throughout the system

Pre-condition: Desired operating pressure and maximum allowable difference are specified

Flow of Events:

1. Pressure sensor takes reading of the operating temperature
2. Sensor compares operating temperature to desired pressure
3. Sensor compares the difference in the actual and desired pressure to the specified allowable difference
4. If the difference is smaller, then alarm does nothing. If it is larger, the alarm goes off.

Post-condition: The appropriate action is taken based on the operating pressure. If there is a dangerous condition, the alarm goes off, if not, then process goes on as normal.

Scenario (2.3): Flow rate

Description: Flow rate sensors detect the difference between the desired operating pressure and the actual operating pressure and alerts if there is a certain difference between the two.

Primary Object: Flow rate sensor

Primary Actors: Streams of reactants and products throughout the system

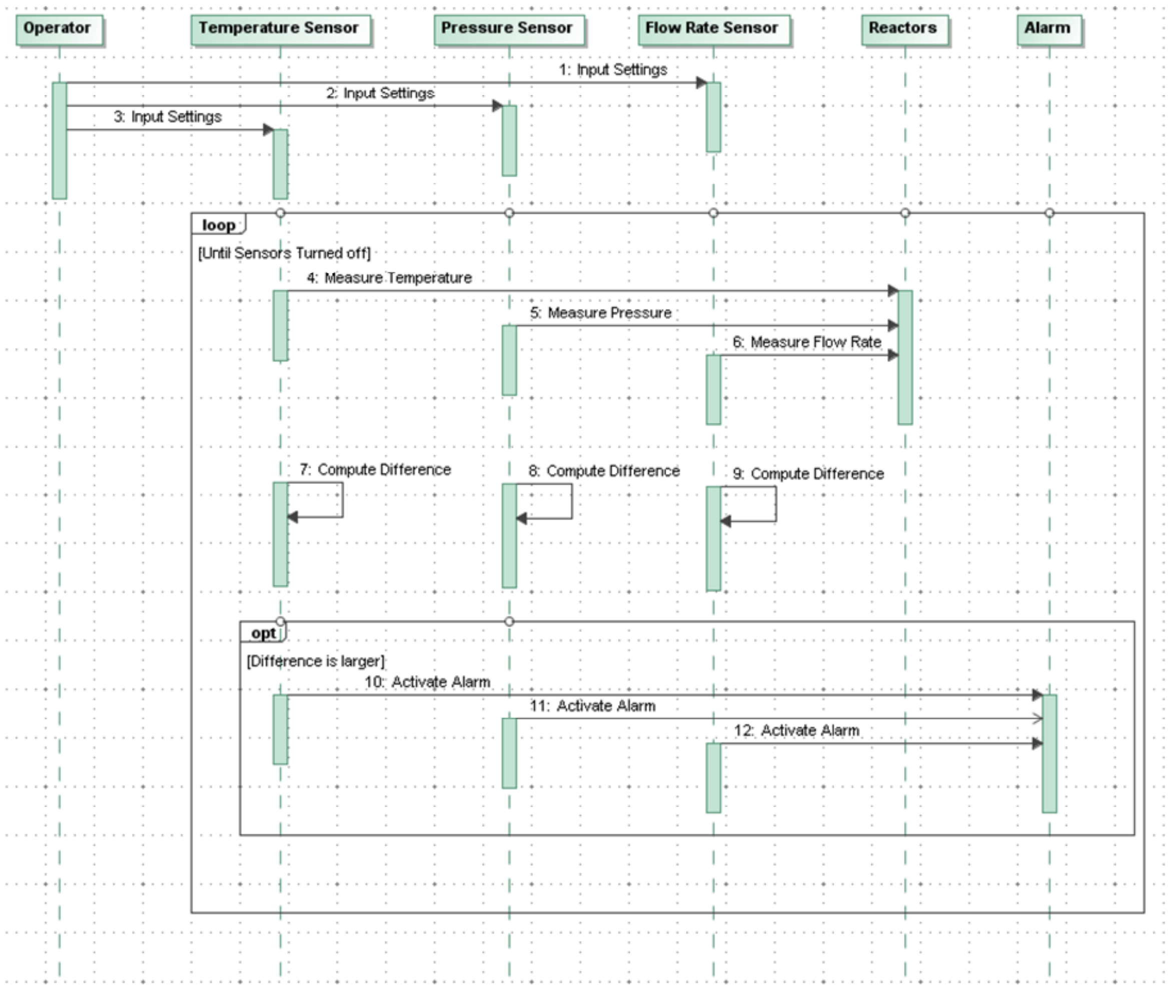
Pre-condition: Desired operating flow rate and maximum allowable difference are specified

Flow of Events:

1. Flow rate sensor takes reading of the operating temperature
2. Sensor compares operating temperature to desired pressure
3. Sensor compares the difference in the actual and desired pressure to the specified allowable difference
4. If the difference is smaller, then alarm does nothing. If it is larger, the alarm goes off.

Post-condition: The appropriate action is taken based on the operating pressure. If there is a dangerous condition, the alarm goes off, if not, then process goes on as normal.

Sequence Diagram for Use Case 2



Use Case 3: Maintenance

The third use case addresses the need to perform regular maintenance and inspections on the plant and ensure the process is operating properly. The maintenance operator should be able to inspect each reactor and the sensors and piping attached to them. The operator will proceed with each reactor in sequence and the equipment attached to them. If there is a problem appropriate actions should be taken to rectify the problem. In the end the time and date of maintenance should be documented to verify that everything is working as it should. The number of different possibilities for maintenance issues is too large to comprehensively cover, but the following scenarios address common/simplified possibilities:

Scenario (3.1): Reactor Maintenance

Description: Reactors will be inspected for performance

Primary Object: Reactors

Primary Actors: Maintenance Operator

Pre-condition: Process is not running

Flow of Events:

1. Operator inspects the reactor for any signs of problems
2. If there is a problem, the operator will take appropriate action, whether it is replacing or fixing the reactor/problem
3. The operator documents the actions taken and the date the inspection took place

Post-condition: Reactor is ready for optimal performance.

Scenario (3.1.1): Weakened Structural Integrity

Description: Structural weakening in reactors must be detected and replaced

Primary Object: Reactor

Primary Actors: Maintenance Operator

Pre-condition: Process not running

Flow of Events:

1. Maintenance operator inspects reactor
2. Operator discovers structural weakness, such as corrosion from HCl
3. Reactor is removed and replaced with new reactor
4. Maintenance is documented

Post-condition: New reactor installed and process is able to continue without increased operation hazard levels

Scenario (3.1.2): Leak in Reactor

Description: Reactor develops a leak and must be patched up or replaced

Primary Object: Reactor

Primary Actors: Maintenance Operator

Pre-condition: Process not running

Flow of Events:

1. Maintenance operator inspects reactor
2. Detects leak, most likely through a pressure test
3. Operator determines if leak can be fix through patching or replacement is immediately necessary
4. Reactor is either fixed or replaced according to the need
5. Maintenance is documented

Post-condition: Leak is fixed, and process is able to continue without increased operation hazard levels

Scenario (3.2): Sensor and Piping Maintenance

Description: Sensors and pipes will be inspected for performance

Primary Object: Sensors

Primary Actors: Maintenance Operator

Pre-condition: Process is not running

Flow of Events:

1. Operator inspects the sensor for any signs of problems as well as proper settings
2. Operator inspects the pipes for build-up or clogs or weaknesses
3. If there is a problem, the operator will take appropriate action, whether it is replacing the sensor/pipes or fixing the settings
4. The operator documents the actions taken and the date the inspection took place

Post-condition: Sensor and pipes are ready for optimal performance.

Scenario (3.1.2): Temperature Sensor Maintenance

Description: Temperature Sensor tested for accuracy and performance

Primary Object: Temperature Sensor

Primary Actors: Maintenance Operator

Pre-condition: Process not running

Flow of Events:

1. Maintenance operator inspects temperature sensor, testing its capability to detect known temperatures within the acceptable accuracy and its ability to determine the correct course of action based on what it senses
2. Temperature sensor is recalibrated or replaced if not detecting the correct temperature or taking the right action after detecting temperature
3. Maintenance is documented

Post-condition: Temperature sensor is able to detect the correct temperature within the specified accuracy and able to take the correct course of action based on its readings and process is able to continue without increased operation hazard levels

Scenario (3.1.2): Piping Leak Maintenance

Description: Pipe tested for leaks

Primary Object: Reactor Piping

Primary Actors: Maintenance Operator

Pre-condition: Process not running

Flow of Events:

1. Maintenance operator inspects pipes for leaks, most likely by running pressure or flow tests
2. Any presence of leaks is detected and their severity determined
3. If problem is sever, pipe may have to be replaced immediately, if it is minor, patching of pipe may be acceptable
4. Maintenance is documented

Post-condition: Pipe leak is eliminated and process is able to continue without increased operation hazard levels

Requirements and Traceability

High level requirements & specifications

#	Requirements	Specifications
1	Produce Polysilicon	>1000MTA
2	Minimize TET waste	<1MTA
3	Produce SiO_2	>3000MTA
4	Produce a profit	10% return on investment over 10 years
5	Produce high quality Poly-Si	>99.9999% purity
6	Produce high quality SiO_2	>97% purity

Derived requirements & traceabiulity

Use Case	Scenario	Req. #	Description
Reaction of input to form output	1.1	1.1.1	MG-Si must react with HCl to for TCS
	1.1	1.1.2	Vapor must pass through top of FBR
	1.1	1.1.3	Solid wastes must exit through bottom of FBR
	1.2	1.2.1	Vapor from FBR must be separated into desirables and undesirables
	1.2.1	1.2.2	All H_2 is removed from stream
	1.2.2	1.2.3	All BCl_3 is removed from stream
	1.2.3	1.2.4	All PCl_5 is removed from stream

	1.2.4	1.2.5	Most TET is separated from TCS
	1.3	1.3.1	TCS reacts with H_2 to form Poly-Si
	1.3	1.3.2	Poly-si is deposited onto seed rods
	1.3	1.3.3	Poly-si is >99.9999% purity
	1.3	1.3.4	Other compounds exit CVD safetly
	1.4	1.4.1	Products from CVD are separated into desirables and undesirables
	1.4.1	1.4.2	Most TET is removed from CVD product stream
	1.4.2	1.4.3	Most HCl is removed from stream
	1.5	1.5.1	TET must react with H2O to form SiO2
	1.5	1.5.2	SiO2 must be >97% purity
	1.5	1.5.3	Most TET from process must be consumed
	1.5.1	1.5.4	SiO2 must exit through bottom of cyclone
	1.5.1	1.5.5	Other compounds exit through top of cyclone

Use Case	**Scenario**	**Req. #**	**Description**

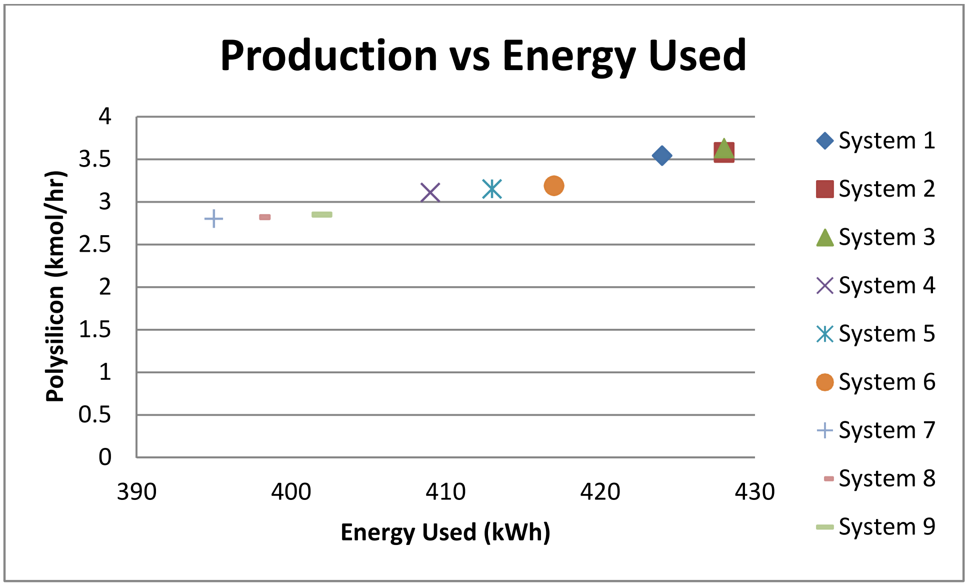
Alarm	2.1	2.1.1	Temperature sensors detect operating temperature within 1 K (Kelvin, not 1000) accuracy
	2.1	2.1.2	Temperature sensors determine difference between operating and desired conditions
	2.1	2.1.3	Temperature sensors take correct action
	2.2	2.2.1	Pressure sensors detect operating pressure within 0.1 bar accuracy
	2.2	2.2.2	Pressure sensors determine difference between operating and desired conditions
	2.2	2.2.3	Pressure sensors take correct action
	2.3	2.3.1	Flow rate sensors detect operating flow rate within
	2.3	2.3.2	Flow rate sensors determine difference between operating and desired conditions
	2.3	2.3.3	Flow Rate sensors take correct action
Maintenance	3.1	3.1.1	Maintenance operator must be able to inspect all aspects of the reactors
	3.1	3.1.2	Reactors should be able to be replaced without dismantling the entire plant
	3.2	3.2.1	Sensors must be able to be operated apart from the rest of the process
	3.2	3.2.2	Spare sensor and piping parts/equipment should be available

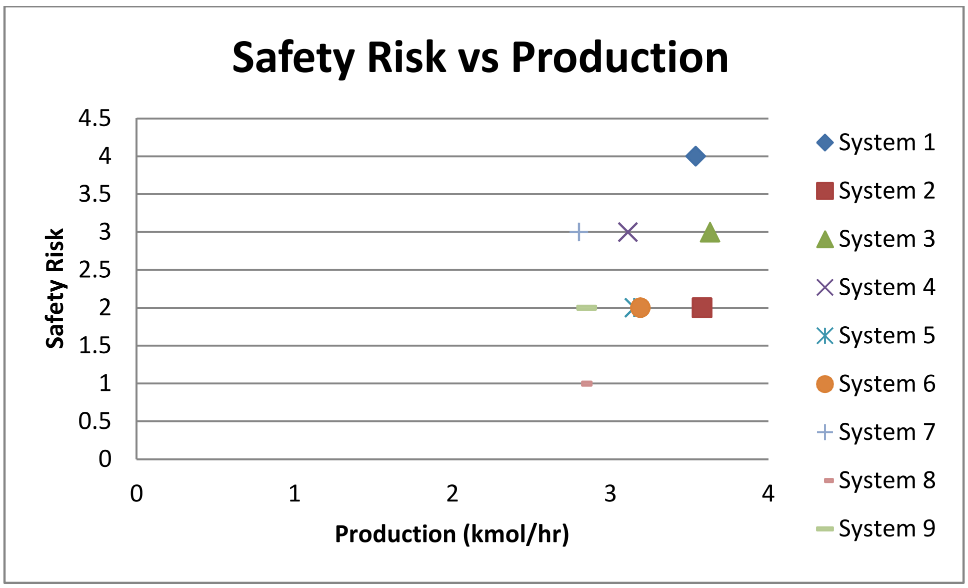
Trade Off Analysis

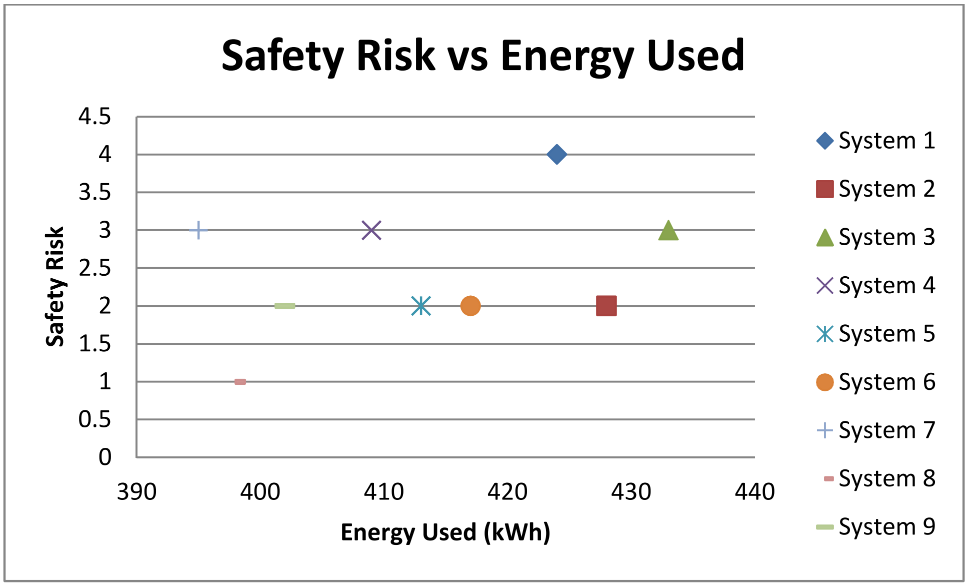
The trade-off analysis focuses on the primary deposition reactor for three system level aspects: energy used,polysilicon production, and safety. The focus on the deposition reactor is due to its possession of the greatest variability in results and is the entire purpose of the entire system. For the design in the trade-off analysis, operating condition variables of temperature and pressure were chosen and their effect on the energy used, production, and safety was assessed. The energy used is the required energy necessary to supplement the reactions that occur. The production is the total amount of solid polysilicon that is produced in the deposition reactor. The relative safety risk is classified from 1 to 4 where pressure is the primary consideration of risk with operating temperature as a secondary risk. The table below displays the quantitative values of specified operating variables and conditions.

System Number	Operating Temperature (K)	Operating Pressure (bar)	Energy Used (kWh)	Production (kmol/hr)	Relative Safety Risk
1	1373	1.1	424	3.54	4
2	1373	1	428	3.58	2
3	1373	0.9	433	3.63	3
4	1273	1.1	409	3.11	3
5	1273	1	413	3.15	2
6	1273	0.9	417	3.19	2
7	1173	1.1	395	2.80	3
8	1173	1	398	2.82	1
9	1173	0.9	402	2.85	2

Possible combinations of systems arrangements were based on variations in temperature and pressure. There are many possible combinations of operating temperatures and pressure. For the purposes of this report, only 3 different temperatures and 3 different pressures are considered. In order to carry out the tradeoff analysis, the graphs of the 3 system level aspects are plotted.


Production vs Energy Used
Polysilicon (kmol/hr)
4
3.5
3
2.5
2
1.5
1
0.5
0
390
400
410
420
430
Energy Used (kWh)
System 1
System 2
System 3
System 4
System 5
System 6
System 7
System 8
System 9


Safety Risk vs Production
Safety Risk
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
0
1
2
3
4
Production (kmol/hr)
System 1
System 2
System 3
System 4
System 5
System 6
System 7
System 8
System 9



Graph Analysis

The graphs show each system as a point of interest that can be considered more thoroughly to determine an optimal setting. For the safety risk factor and the amount of energy used, it is desirable to be closer to the origin for optimal placement of points. For the production of polysilicon, it is ideal to be further away from the origin for optimal placement of points.

From the Production vs. Energy Used graph, there is a very distinct and clear trend. As the amount of energy used increases, so does the amount of polysilicon produced. While the graph appears to show a very distance and large difference in the amount of energy used in order to produce more polysilicon, it can be seen that the difference in energy used between system 4 and system 2 is only 8% higher whereas the difference in production is a significant 27% increase in production. With this, it is clear that from a very distinct trend associated between energy consumed by the reactor and the production amount that a higher energy consumption rate is ideal as the production quantity of polysilicon is increased at a much larger quantity.

Next, the safety risk vs production graph is considered. There is no clear trend between the safety risk of the deposition reactor and the production quantity. In addition, a higher production rate naturally increases the operating conditions of the deposition reactor resulting in higher safety risk. In effort to minimize the safety risks of the process while maintaining as large production as possible, systems 8 and system 2 are reasonable candidates for consideration.

Lastly, the safety risk vs energy graph is considered. Again, there is no clear trend between the safety risk and the consumption of energy. There is also no direct connection between an increase in energy consumption and safety risk. Due to many systems having relatively low safety risks, the ones with the lowest energy use are system 8 and system 9.

In order to find the best combination of design variables, a consideration of all 3 graphs is necessary. However, at the present time, energy costs are valued at a very low \$0.06/kWh. Because of this allowance, focus will not be placed on the safety risk vs energy graph. From the remaining graph analysis, an overlap of optimal systems is obtained for system 8 and system 2. While system 8 has the lowest safety risk, the large increase in polysilicon production can be justified and the risk assessed to prevent accidents.

Financials

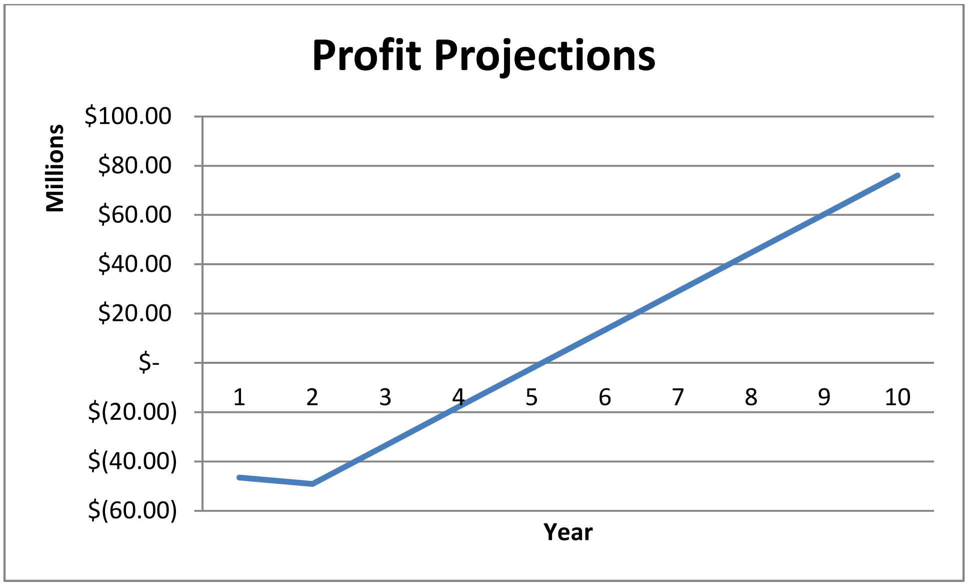
The fixed costs of all process equipment are calculated via chemcad or obtained by industry standards.

		Fixed Installed Cost
Distillation Column 3	$	1,300,000.00
Distillation Column 6	$	1,300,000.00
Distillation Column 17	$	1,000,000.00
Distillation Column 18	$	1,400,000.00
Distillation Column 19	$	1,400,000.00
Cyclone 9	$	1,500.00
Cylone 10	$	1,500.00
FBR	$	39,000.00
FBR Separator	$	3,200.00
FBR Separator 2	$	5,000.00
CVD	$	40,000,000.00
Hydrolysis Reactor	$	115,000.00
SUMMATION	$	46,565,200.00

Variable costs are calculated via the input and output of the system as well as tacking on additional overhead such as tax on revenue and 325 day operation.

Energy Cost	$ 20,738,473.57
Silicon	46526789.84
SiO2	19850899.66
Current Consumption	
H2	-329664
HCl	-45496.37474
H2O	-3299.649408
Mg Si	-8883302.4
Operating Running	
Total	36,377,453.50

This leads to an overall economic forecast indicated by the graph below: The first year is forecasted to be complete installation of the facility. The second year is taken to be half capacity and only by third year is full capacity in effect. This returns a return on investment of 66% allowing for additional consideration in safety of system performance as well as other miscellaneous costs not taken into account by an elementary financial analysis.



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Appendix I: ChemCAD Data

CHEMCAD 6.0.1 Page 1

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

FLOWSHEET SUMMARY

Equipment	Label	Stream Numbers
1	REAC	3 -4
2	CSEP	4 -5 -6
3	SCDS	35 -7 -8
4	GIBS	33 -2
5	CSEP	2 -21 -22
6	SCDS	22 -32 -24
7	MIXE	8 24 11 -12
8	REAC	12 -10
9	CYCL	10 -13 -14
10	CYCL	13 -18 -19
12	MIXE	7 5 9 -1
13	CYCL	15 -16 -17
14	MIXE	14 19 -20
16	SCDS	6 -30 -31
17	SCDS	32 -29 -23
18	MIXE	1 23 -33
19	SCDS	31 -35 -34

Stream Connections

Stream	Equipment		Stream	Equipment		Stream	Equipment	
	From	To		From	To		From	To
1	12	18	12	7	8	23	17	18
2	4	5	13	9	10	24	6	7
3		1	14	9	14	29	17	
4	1	2	15		13	30	16	
5	2	12	16	13		31	16	19
6	2	16	17	13		32	6	17
7	3	12	18	10		33	18	4
8	3	7	19	10	14	34	19	
9		12	20	14		35	19	3
10	8	9	21	5				
11		7	22	5	6			

Calculation mode : Sequential
Flash algorithm : Normal

Equipment Calculation Sequence
1 2 13 16 19 3 12 18 4 5 6 17 7 8 9 10 14

Equipment Recycle Sequence
18 4 5 6 17

Recycle Cut Streams

23

CHEMCAD 6.0.1 Page 2

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

Recycle Convergence Method: Direct Substitution

Max. loop iterations 40

Recycle Convergence Tolerance

Flow rate	1.000E-003
Temperature	1.000E-003
Pressure	1.000E-003
Enthalpy	1.000E-003
Vapor frac.	1.000E-003

Recycle calculation has converged.

Run Time Error and Warning Messages:

*** Equip. 19 ***

Can't converge with original specs. Alternative optimal solution is found.

* Uop 12, Check mass balance.

CHEMCAD 6.0.1 Page 3

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

Overall Mass Balance	kmol/h		kg/h	
	Input	Output	Input	Output
Hydrogen	10.000	26.571	20.158	53.561
Dichlorosilane	0.000	0.015	0.000	1.505
Trichlorosilane	0.000	0.160	0.000	21.729
Silicon TetraCl	0.000	0.126	0.000	21.344
Hydrogen Chlorid	39.690	37.694	1447.137	1374.361
Silicon	12.600	4.055	353.871	113.884
Water	18.840	3.008	339.403	54.182
Silicon Dioxide	2.575	10.491	154.716	630.354
Boron Trichlorid	0.008	0.008	0.903	0.899
Phosphoric Chlor	0.008	0.008	1.606	1.606
Total	83.720	82.135	2317.795	2273.425

Warning: Overall mass balance not good enough. Need lower flow tolerance.

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

COMPONENTS

	ID #	Name	Formula	
1	1	Hydrogen	H2	
2	935	Dichlorosilane	H2Cl2Si	
3	938	Trichlorosilane	HCl3Si	
4	944	Silicon TetraCl	Cl4Si	
5	104	Hydrogen Chlorid	HCl	
6	993	Silicon	Si	* solid *
7	62	Water	H2O	
8	987	Silicon Dioxide	O2Si	* solid *
9	629	Boron Trichlorid	BCl3	
10	946	Phosphoric Chlor	Cl5P	

THERMODYNAMICS

K-value model : Henry's law
Enthalpy model : Latent Heat
Liquid density : Library

Std vapor rate reference temperature is 0 C.
Atmospheric pressure is 1.0132 bar.

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

EQUIPMENT SUMMARIES

Reactor Summary

Equip. No.	1	8
Name		
Thermal mode	2	2
Temperature K	623.0000	573.0000
Heat duty kW	-802.9692	1391.8734
Key Component	6	4
Frac. Conversion	1.0000	0.9990
Reactor Pressure bar	1.0000	
Calc H of Reac. (kJ/kmol)	-230448.5938	471754.5000
Stoichiometrics:		
Hydrogen	1.150	0.000E+000
Trichlorosilane	0.850	0.000E+000
Silicon TetraCl	0.150	-1.000
Hydrogen Chlori	-3.150	4.000
Silicon	-1.000	0.000E+000
Water	0.000E+000	-2.000
Silicon Dioxide	0.000E+000	1.000

Component Separator Summary

Equip. No.	2	5
Name		
Top Temp Spec	623.0000	1373.0000
Bottom Temp Spec	623.0000	1373.0000
Heat duty kW	0.0001	-69.1435
Component No. 1	1.0000	1.0000
Component No. 6	1.0000	1.0000
Component No. 9		1.0000
Component No. 10		1.0000

Scds Rigorous Distillation Summary

Equip. No.	3	6	16	17
Name				
No. of stages	20	20	20	10
1st feed stage	4	10	11	5
Condenser mode	7	1	7	1
Condenser spec	0.9900	20.0000	0.9950	5.0000
Cond comp i pos.	3	3	9	0
Reboiler mode	7	7	7	7
Reboiler spec.	0.9900	0.9000	0.9950	0.9000
Reboiler comp i	4	4	3	2
Est. dist. rate (kmol/h)	10.6667			2.9630

Est. reflux rate (kmol/h)	24.6230			14.8150

CHEMCAD 6.0.1 Page 6

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

EQUIPMENT SUMMARIES

Est. T top K	304.6428	321.1796	304.3802	188.9737
Est. T bottom K	329.6360	332.2907	315.4913	301.7689
Est. T 2 K	304.6835			189.4986
Calc Cond duty kW	-1087.2502	-1391.5433	-542.2547	-165.2581
Calc Reblr duty kW	1087.7965	936.9020	354.4969	176.9636
Initial flag	6	1	6	1
Calc Reflux mole (kmol/h)	143.7663	188.2681	77.1328	30.2214
Calc Reflux ratio	13.6045	20.0000	1260.2826	5.0000
Calc Reflux mass kg/h	19481.4766	13934.0947	10270.8555	1106.7990
Column diameter m	2.5000	2.5000	2.5000	2.5000
Tray space m	2.4000	2.4000	2.4000	2.4000
Column length m	17.0000	17.0000	21.0000	12.0000
Thickness (top) m	0.0600	0.0600	0.0600	0.0600
Thickness (bot) m	0.0600	0.0600	0.0600	0.0600
Material density (kg/m3)	7850.0000	7850.0000	7850.0000	7850.0000
Actual no of trays	24.0000	24.0000	24.0000	12.0000
Install factor	3.0000	3.0000	3.0000	3.0000
Column purchase $	395090	395090	449095	309574
Column installed $	1185270	1185270	1347286	928722
Cost estimation flag	1	1	1	1
Shell weight kg	70393	70393	85189	51896
Cost of shell $	253702	253702	292580	202779
Cost of trays $	37551	37551	37551	25964
Platform & ladder $	19507	19507	23107	14755
No of sections	1	1	1	1
Condenser area m2	100.0000	100.0000	100.0000	100.0000
Cond P design bar			1.0000	
Reboiler area m2	100.0000	100.0000	100.0000	100.0000
Rebl P design bar			1.0000	
Cond purchase $	15640	15640	15640	15640
Cond installed $	31281	31281	31281	31281
Rebl purchase $	15640	15640	15640	15640
Rebl installed $	31281	31281	31281	31281
Total purchase $	426371	426371	480376	340855
Total installed $	1247831	1247831	1409848	991283
Optimization flag	1	1	1	1
Calc. tolerance	7.9771e-006	0.0005	7.2281e-006	8.4822e-006

*** Equip. 19 ***

Can't converge with original specs. Alternative optimal solution is found.

Equip. No.	19
Name	
No. of stages	20
1st feed stage	10
Condenser mode	7

```
Condenser spec              0.9999
Cond comp i pos.               3
Reboiler mode                  7
Reboiler spec.              0.9999
Reboiler comp i               10
Est. dist. rate            12.4287
```


EQUIPMENT SUMMARIES

```
 (kmol/h)
Est. reflux rate            0.1526
 (kmol/h)
Est. T top  K             307.3199
Est. T bottom  K          556.5712
Est. T 2  K               310.9799
Calc Cond duty  kW        -98.6244
Calc Reblr duty  kW        98.6618
Initial flag                   6
Calc Reflux mole            1.2429
 (kmol/h)
Calc Reflux ratio           0.1000
Calc Reflux mass  kg/h    174.4520
Column diameter  m          2.5000
Tray space  m               2.4000
Column length  m           21.0000
Thickness (top)  m          0.0600
Thickness (bot)  m          0.0600
Material density         7850.0000
 (kg/m3)
Actual no of trays         24.0000
Install factor              3.0000
Column purchase  $          449095
Column installed  $        1347286
Cost estimation flag           1
Shell weight  kg             85189
Cost of shell  $            292580
Cost of trays  $             37551
Platform & ladder  $         23107
No of sections                 1
Condenser area  m2        100.0000
Cond P design  bar          1.0000
Reboiler area  m2         100.0000
Rebl P design  bar          1.0000
Cond purchase  $             15640
Cond installed  $            31281
Rebl purchase  $             15640
Rebl installed  $            31281
Total purchase  $           480376
Total installed  $         1409848
Optimization flag              1
Calc. tolerance        5.5649e-007
```

Gibbs Reactor Summary

Equip. No.	4
Name	
Thermal mode	2
Reaction Phase	1
Temperature K	1373.0000
Heat duty kW	815.0995
Pressure bar	1.0000
Overall Heat of Rxn	89.3146

EQUIPMENT SUMMARIES

(kW)	
Solid Component	6

Mixer Summary

Equip. No.	7	12	14	18
Name				
Output Pressure bar	1.1000			

Cyclone Summary

Equip. No.	9	10	13
Name			
Vane constant	16.0000	16.0000	16.0000
Cyclone diameter m	0.1000	0.1000	0.1000
No. of cyclones	5.0000	1.0000	1.0000
Inlet height m	0.0500	0.0500	0.0500
Inlet width m	0.0200	0.0200	0.0200
Outlet length m	0.0500	0.0500	0.0500
Outlet diameter m	0.0500	0.0500	0.0500
Cylinder height m	0.1500	0.1500	0.1500
Overall length m	0.4000	0.4000	0.4000
Dust outlet dia. m	0.0375	0.0375	0.0375
No. of gas turns	5.0000	5.0000	5.0000
Overall efficiency	0.9992	1.0000	9.9793e-031
Pressure drop bar	0.1598	4.6717	0.0190
Std gas flow m3/h	712.6849	712.6849	67.0168
Cost estimation flag	1	1	1
Purchase cost $	754	754	74
Installed cost $	1056	1056	104

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STREAM PROPERTIES

Stream No.	1	2	3	4
Name				
- - Overall - -				
Molar flow kmol/h	34.7295	45.3726	52.3054	27.1054
Mass flow kg/h	1436.9562	1912.3660	1803.5179	1803.4990
Temp K	268.5774	1373.0000	623.0000	623.0000
Pres bar	1.0000	1.0000	1.0000	1.0000
Vapor mole fraction	0.9237	1.000	1.000	1.000
Enth kW	-1448.7	-1146.9	-887.53	-1690.5
Tc K	315.4425	329.0780	325.4156	388.5290
Pc bar	126.1360	151.3810	84.1843	114.7742
Std. sp gr. wtr = 1	0.831	0.904	0.969	1.057
Std. sp gr. air = 1	1.429	1.455	1.191	2.297
Degree API	38.7980	25.0419	14.5571	2.3324
Average mol wt	41.3757	42.1480	34.4805	66.5365
Actual dens kg/m3	2.0102	0.4013	0.8771	1.2851
Actual vol m3/h	714.8267	4765.2368	2056.1179	1403.4258
Std liq m3/h	1.7294	2.1157	1.8616	1.7058
Std vap 0 C m3/h	778.4144	1016.9653	1172.3553	607.5314
- - Vapor only - -				
Molar flow kmol/h	32.0786	41.7357	39.7054	27.1054
Mass flow kg/h	1077.7009	1810.2236	1449.6469	1803.4990
Average mol wt	33.5956	43.3735	36.5100	66.5365
Actual dens kg/m3	1.5082	0.3799	0.7051	1.2851
Actual vol m3/h	714.5700	4765.1926	2055.9654	1403.4258
Std liq m3/h	1.4643	2.0718	1.7097	1.7058
Std vap 0 C m3/h	718.9994	935.4489	889.9433	607.5314
Cp kJ/kg-K	1.1613	1.1445	0.8128	0.8963
Z factor	0.9977	1.0003	0.9998	0.9997
Visc N-s/m2	1.171e-005	4.713e-005	2.929e-005	2.368e-005
Th cond W/m-K	0.0692	0.1696	0.0291	0.0742
- - Liquid only - -				
Molar flow kmol/h	2.6508			
Mass flow kg/h	359.2552			
Average mol wt	135.5249			
Actual dens kg/m3	1399.5706			
Actual vol m3/h	0.2567			
Std liq m3/h	0.2651			
Std vap 0 C m3/h	59.4151			
Cp kJ/kg-K	0.8817			
Z factor	0.0045			
Visc N-s/m2	0.0004351			
Th cond W/m-K	0.1351			
Surf tens N/m	0.0213			

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

STREAM PROPERTIES

Stream No.	5	6	7	8
Name				
- - Overall - -				
Molar flow kmol/h	14.4900	12.6154	10.5676	1.8611
Mass flow kg/h	29.2090	1774.2902	1431.9910	312.5285
Temp K	623.0000	623.0000	304.6457	327.7168
Pres bar	1.0000	1.0000	1.0000	1.0000
Vapor mole fraction	1.000	1.000	0.0000	0.0000
Enth kW	35.555	-1726.1	-1530.4	-350.78
Tc K	33.2700	484.2731	479.0571	505.6690
Pc bar	12.9595	41.3810	41.6966	36.3671
Std. sp gr. wtr = 1	0.070	1.377	1.355	1.486
Std. sp gr. air = 1	0.070	4.856	4.679	5.798
Degree API	1889.9269	-28.7418	-27.0585	-36.2954
Average mol wt	2.0158	140.6445	135.5077	167.9283
Actual dens kg/m3	0.0389	2.7248	1311.9866	1400.1318
Actual vol m3/h	750.7029	651.1588	1.0915	0.2232
Std liq m3/h	0.4173	1.2885	1.0570	0.2103
Std vap 0 C m3/h	324.7737	282.7577	236.8584	41.7137
- - Vapor only - -				
Molar flow kmol/h	14.4900	12.6154		
Mass flow kg/h	29.2089	1774.2902		
Average mol wt	2.0158	140.6445		
Actual dens kg/m3	0.0389	2.7248		
Actual vol m3/h	750.7029	651.1588		
Std liq m3/h	0.4173	1.2885		
Std vap 0 C m3/h	324.7737	282.7577		
Cp kJ/kg-K	14.5508	0.6716		
Z factor	1.0003	0.9966		
Visc N-s/m2	1.479e-005	2.234e-005		
Th cond W/m-K	0.3021	0.0210		
- - Liquid only - -				
Molar flow kmol/h			10.5676	1.8611
Mass flow kg/h			1431.9910	312.5285
Average mol wt			135.5077	167.9283
Actual dens kg/m3			1311.9866	1400.1318
Actual vol m3/h			1.0915	0.2232
Std liq m3/h			1.0570	0.2103
Std vap 0 C m3/h			236.8584	41.7137
Cp kJ/kg-K			0.9387	0.8393
Z factor			0.0042	0.0047
Visc N-s/m2			0.0003086	0.0003489
Th cond W/m-K			0.1232	0.0966
Surf tens N/m			0.0166	0.0157

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

STREAM PROPERTIES

Stream No.	9	10	11	12
Name				
- - Overall - -				
Molar flow kmol/h	10.0000	39.7131	15.8500	23.8807
Mass flow kg/h	20.1580	1646.2687	285.5377	1646.2845
Temp K	305.0000	573.0000	298.0000	313.2391
Pres bar	1.0000	1.1000	1.0000	1.1000
Vapor mole fraction	1.000	1.000	0.0000	0.0000
Enth kW	-1.2754	-1395.9	-1257.9	-2787.7
Tc K	33.2700	326.6678	647.3500	545.8163
Pc bar	12.9595	85.1165	221.1823	53.6634
Std. sp gr. wtr = 1	0.070	1.060	1.000	1.374
Std. sp gr. air = 1	0.070	1.431	0.622	2.380
Degree API	1889.9286	2.0210	10.0000	-28.5509
Average mol wt	2.0158	41.4540	18.0150	68.9378
Actual dens kg/m3	0.0795	1.1960	996.7463	1333.3728
Actual vol m3/h	253.6836	1376.5118	0.2865	1.2347
Std liq m3/h	0.2880	1.5534	0.2855	1.1978
Std vap 0 C m3/h	224.1365	890.1160	355.2563	535.2539
- - Vapor only - -				
Molar flow kmol/h	10.0000	31.7969		
Mass flow kg/h	20.1580	1170.6313		
Average mol wt	2.0158	36.8159		
Actual dens kg/m3	0.0795	0.8505		
Actual vol m3/h	253.6836	1376.3304		
Std liq m3/h	0.2880	1.3739		
Std vap 0 C m3/h	224.1365	712.6849		
Cp kJ/kg-K	14.2970	0.8069		
Z factor	1.0005	0.9996		
Visc N-s/m2	9.005e-006	2.721e-005		
Th cond W/m-K	0.1749	0.0269		
- - Liquid only - -				
Molar flow kmol/h			15.8500	23.8807
Mass flow kg/h			285.5377	1646.2845
Average mol wt			18.0150	68.9378
Actual dens kg/m3			996.7463	1333.3727
Actual vol m3/h			0.2865	1.2347
Std liq m3/h			0.2855	1.1978
Std vap 0 C m3/h			355.2563	535.2539
Cp kJ/kg-K			4.1851	1.4097
Z factor			0.0010	0.0025
Visc N-s/m2			0.0009258	0.0005661
Th cond W/m-K			0.6060	0.1520
Surf tens N/m			0.0721	0.0250

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STREAM PROPERTIES

Stream No.	13	14	15	16
Name				
- - Overall - -				
Molar flow kmol/h	31.8036	7.9096	5.5650	5.5650
Mass flow kg/h	1171.0302	475.2384	208.5811	208.5811
Temp K	572.6719	572.6719	573.0000	572.9728
Pres bar	0.9402	0.9402	1.0000	0.9810
Vapor mole fraction	1.000	0.0000	1.000	1.000
Enth kW	-758.27	-637.60	-400.45	-400.45
Tc K	326.6678	0.0000	647.3500	647.3500
Pc bar	85.1165	0.0000	221.1823	221.1823
Std. sp gr. wtr = 1	0.852	2.649	1.858	1.858
Std. sp gr. air = 1	1.271	2.075	1.294	1.294
Degree API	34.5318	-78.0883	-55.3400	-55.3400
Average mol wt	36.8207	60.0840	37.4809	37.4809
Actual dens kg/m3	0.7276	2621.5273	1.4673	1.4394
Actual vol m3/h	1609.4430	0.1813	142.1554	144.9038
Std liq m3/h	1.3741	0.1794	0.1123	0.1123
Std vap 0 C m3/h	712.8336	177.2822	124.7319	124.7319
- - Vapor only - -				
Molar flow kmol/h	31.7969		2.9900	2.9900
Mass flow kg/h	1170.6313		53.8648	53.8648
Average mol wt	36.8159		18.0150	18.0150
Actual dens kg/m3	0.7274		0.3791	0.3719
Actual vol m3/h	1609.4428		142.0963	144.8448
Std liq m3/h	1.3739		0.0539	0.0539
Std vap 0 C m3/h	712.6849		67.0168	67.0168
Cp kJ/kg-K	0.8069		2.0002	2.0001
Z factor	0.9996		0.9977	0.9977
Visc N-s/m2	2.719e-005		2.034e-005	2.034e-005
Th cond W/m-K	0.0268		0.0436	0.0436
- - Liquid only - -				
Molar flow kmol/h				
Mass flow kg/h				
Average mol wt				
Actual dens kg/m3				
Actual vol m3/h				
Std liq m3/h				
Std vap 0 C m3/h				
Cp kJ/kg-K				
Z factor				
Visc N-s/m2				
Th cond W/m-K				
Surf tens N/m				

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STREAM PROPERTIES

Stream No.	17	18	19	20
Name				
- - Overall - -				
Molar flow kmol/h	0.0000	31.7969	0.0066	7.9162
Mass flow kg/h	0.0000	1170.6312	0.3989	475.6373
Temp K	0.0000	509.4411	509.4411	572.6204
Pres bar	0.0000	0.0000	0.0000	0.9402
Vapor mole fraction	0.0000	1.000	0.0000	0.0000
Enth kW	0.00000	-755.82	-0.54234	-638.15
Tc K	0.0000	326.6678	0.0000	0.0000
Pc bar	0.0000	85.1165	0.0000	0.0000
Std. sp gr. wtr = 1	0.000	0.852	2.649	2.649
Std. sp gr. air = 1	0.000	1.271	2.075	2.075
Degree API	0.0000	34.5702	-78.0883	-78.0883
Average mol wt	0.0000	36.8159	60.0840	60.0840
Actual dens kg/m3	0.0000	0.0000	2627.6962	2621.5322
Actual vol m3/h	0.0000	1953126643012.5496	0.0002	0.1814
Std liq m3/h	0.0000	1.3739	0.0002	0.1795
Std vap 0 C m3/h	0.0000	712.6849	0.1488	177.4310
- - Vapor only - -				
Molar flow kmol/h		31.7969		
Mass flow kg/h		1170.6312		
Average mol wt		36.8159		
Actual dens kg/m3		0.0000		
Actual vol m3/h		1953126643012.5496		
Std liq m3/h		1.3739		
Std vap 0 C m3/h		712.6849		
Cp kJ/kg-K		0.8023		
Z factor		1.0000		
Visc N-s/m2		2.449e-005		
Th cond W/m-K		0.0240		
- - Liquid only - -				
Molar flow kmol/h				
Mass flow kg/h				
Average mol wt				
Actual dens kg/m3				
Actual vol m3/h				
Std liq m3/h				
Std vap 0 C m3/h				
Cp kJ/kg-K				
Z factor				
Visc N-s/m2				
Th cond W/m-K				
Surf tens N/m				

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STREAM PROPERTIES

Stream No.	21	22	23	24
Name				
- - Overall - -				
Molar flow kmol/h	30.6257	15.5830	3.3691	6.1696
Mass flow kg/h	167.4450	1744.9207	475.3427	1048.2182
Temp K	1373.0000	1373.0000	306.8699	329.7928
Pres bar	1.0000	1.0000	1.0000	1.0000
Vapor mole fraction	1.000	1.000	0.0000	0.0000
Enth kW	327.46	-1437.9	-513.23	-1179.1
Tc K	33.2700	474.9816	484.6973	507.0000
Pc bar	12.9595	92.8192	41.3092	35.9001
Std. sp gr. wtr = 1	0.206	1.335	1.381	1.493
Std. sp gr. air = 1	0.189	3.866	4.871	5.866
Degree API	556.4040	-25.5211	-29.0032	-36.7433
Average mol wt	5.4675	111.9758	141.0886	169.8996
Actual dens kg/m3	0.0552	0.9806	1333.7551	1403.6521
Actual vol m3/h	3033.3404	1779.4601	0.3564	0.7468
Std liq m3/h	0.8140	1.3069	0.3443	0.7019
Std vap 0 C m3/h	686.4335	349.2722	75.5140	138.2840
- - Vapor only - -				
Molar flow kmol/h	26.5707	15.5830		
Mass flow kg/h	53.5614	1744.9207		
Average mol wt	2.0158	111.9758		
Actual dens kg/m3	0.0177	0.9806		
Actual vol m3/h	3033.2909	1779.4601		
Std liq m3/h	0.7652	1.3069		
Std vap 0 C m3/h	595.5469	349.2722		
Cp kJ/kg-K	15.7528	0.6952		
Z factor	1.0002	1.0005		
Visc N-s/m2	2.571e-005	4.613e-005		
Th cond W/m-K	0.5482	0.0093		
- - Liquid only - -				
Molar flow kmol/h			3.3691	6.1696
Mass flow kg/h			475.3427	1048.2182
Average mol wt			141.0886	169.8996
Actual dens kg/m3			1333.7551	1403.6521
Actual vol m3/h			0.3564	0.7468
Std liq m3/h			0.3443	0.7019
Std vap 0 C m3/h			75.5140	138.2840
Cp kJ/kg-K			0.9255	0.8332
Z factor			0.0043	0.0048
Visc N-s/m2			0.0003193	0.0003495
Th cond W/m-K			0.1175	0.0954
Surf tens N/m			0.0166	0.0156

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

STREAM PROPERTIES

Stream No.	29	30	31	32
Name				
- - Overall - -				
Molar flow kmol/h	6.0443	0.0612	12.5542	9.4134
Mass flow kg/h	221.3598	8.1497	1766.1406	696.7025
Temp K	189.0152	301.2649	307.3381	196.5361
Pres bar	1.0000	1.0000	1.0000	1.0000
Vapor mole fraction	0.0000	0.0000	0.0000	0.0000
Enth kW	-188.52	-8.6615	-1905.1	-713.46
Tc K	325.5240	477.0123	484.3055	429.9205
Pc bar	83.9184	42.1520	41.3755	124.3196
Std. sp gr. wtr = 1	0.849	1.353	1.377	1.152
Std. sp gr. air = 1	1.264	4.598	4.857	2.555
Degree API	35.0974	-26.9336	-28.7501	-8.6368
Average mol wt	36.6231	133.1581	140.6810	74.0119
Actual dens kg/m3	1191.9519	1319.1171	1328.6638	1421.0085
Actual vol m3/h	0.1857	0.0062	1.3293	0.4903
Std liq m3/h	0.2606	0.0060	1.2825	0.6049
Std vap 0 C m3/h	135.4742	1.3718	281.3859	210.9882
- - Liquid only - -				
Molar flow kmol/h	6.0443	0.0612	12.5542	9.4134
Mass flow kg/h	221.3598	8.1497	1766.1406	696.7025
Average mol wt	36.6231	133.1581	140.6810	74.0119
Actual dens kg/m3	1191.9518	1319.1171	1328.6638	1421.0084
Actual vol m3/h	0.1857	0.0062	1.3293	0.4903
Std liq m3/h	0.2606	0.0060	1.2825	0.6049
Std vap 0 C m3/h	135.4742	1.3718	281.3859	210.9882
Cp kJ/kg-K	1.7587	0.9535	0.9220	1.1149
Z factor	0.0022	0.0042	0.0043	0.0036
Visc N-s/m2	0.0001855	0.0003136	0.0003171	0.0003657
Th cond W/m-K	0.4057	0.1217	0.1180	0.2159
Surf tens N/m	0.0275	0.0169	0.0165	0.0287

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

STREAM PROPERTIES

Stream No.	33	34	35
Name			
- - Overall - -			
Molar flow kmol/h	38.0988	0.1255	12.4287
Mass flow kg/h	1912.3270	21.6210	1744.5196
Temp K	270.4577	330.7219	307.1727
Pres bar	1.0000	1.0000	1.0000
Vapor mole fraction	0.8535	0.0000	0.0000
Enth kW	-1962.0	-23.338	-1881.8
Tc K	345.5220	529.0084	483.7114
Pc bar	123.2367	40.6720	41.2886
Std. sp gr. wtr = 1	0.922	1.418	1.377
Std. sp gr. air = 1	1.733	5.946	4.846
Degree API	21.9438	-31.7208	-28.7133
Average mol wt	50.1939	172.2211	140.3624
Actual dens kg/m3	2.6203	1334.5066	1328.4592
Actual vol m3/h	729.7993	0.0162	1.3132
Std liq m3/h	2.0737	0.0152	1.2672
Std vap 0 C m3/h	853.9326	2.8139	278.5720
- - Vapor only - -			
Molar flow kmol/h	32.5162		
Mass flow kg/h	1141.6558		
Average mol wt	35.1104		
Actual dens kg/m3	1.5655		
Actual vol m3/h	729.2512		
Std liq m3/h	1.5098		
Std vap 0 C m3/h	728.8071		
Cp kJ/kg-K	1.1278		
Z factor	0.9975		
Visc N-s/m2	1.173e-005		
Th cond W/m-K	0.0674		
- - Liquid only - -			
Molar flow kmol/h	5.5826	0.1255	12.4287
Mass flow kg/h	770.6712	21.6210	1744.5196
Average mol wt	138.0497	172.2211	140.3624
Actual dens kg/m3	1405.9118	1334.5066	1328.4592
Actual vol m3/h	0.5482	0.0162	1.3132
Std liq m3/h	0.5640	0.0152	1.2672
Std vap 0 C m3/h	125.1256	2.8139	278.5720
Cp kJ/kg-K	0.8789	0.8202	0.9233
Z factor	0.0045	0.0063	0.0043
Visc N-s/m2	0.0004355	0.0003515	0.0003166
Th cond W/m-K	0.1314	0.0966	0.1183
Surf tens N/m	0.0210	0.0135	0.0165

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

FLOW SUMMARIES

Stream No.	1	2	3	4
Stream Name				
Temp K	268.5774	1373.0000	623.0000	623.0000
Pres bar	1.0000	1.0000	1.0000	1.0000
Enth kW	-1448.7	-1146.9	-887.53	-1690.5
Vapor mole fraction	0.92367	1.0000	1.0000	1.0000
Total kmol/h	34.7295	45.3726	52.3054	27.1054
Flowrates in kmol/h				
Hydrogen	24.4900	27.2689	0.0000	14.4900
Dichlorosilane	0.0000	0.1513	0.0000	0.0000
Trichlorosilane	10.2206	2.6830	0.0000	10.7100
Silicon TetraCl	0.0189	7.1375	0.0000	1.8900
Hydrogen Chlorid	0.0000	4.4949	39.6900	0.0000
Silicon	0.0000	3.6369	12.6000	0.0000
Water	0.0000	0.0000	0.0000	0.0000
Silicon Dioxide	0.0000	0.0000	0.0000	0.0000
Boron Trichlorid	0.0000	0.0000	0.0077	0.0077
Phosphoric Chlor	0.0000	0.0000	0.0077	0.0077

Stream No.	5	6	7	8
Stream Name				
Temp K	623.0000	623.0000	304.6457	327.7168
Pres bar	1.0000	1.0000	1.0000	1.0000
Enth kW	35.555	-1726.1	-1530.4	-350.78
Vapor mole fraction	1.0000	1.0000	0.00000	0.00000
Total kmol/h	14.4900	12.6154	10.5675	1.8611
Flowrates in kmol/h				
Hydrogen	14.4900	0.0000	0.0000	0.0000
Dichlorosilane	0.0000	0.0000	0.0000	0.0000
Trichlorosilane	0.0000	10.7100	10.5498	0.1065
Silicon TetraCl	0.0000	1.8900	0.0177	1.7546
Hydrogen Chlorid	0.0000	0.0000	0.0000	0.0000
Silicon	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.0000	0.0000	0.0000
Silicon Dioxide	0.0000	0.0000	0.0000	0.0000
Boron Trichlorid	0.0000	0.0077	0.0000	0.0000
Phosphoric Chlor	0.0000	0.0077	0.0000	0.0000

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FLOW SUMMARIES

Stream No.	9	10	11	12
Stream Name				
Temp K	305.0000	573.0000	298.0000	313.2391
Pres bar	1.0000	1.1000	1.0000	1.1000
Enth kW	-1.2754	-1395.9	-1257.9	-2787.7
Vapor mole fraction	1.0000	1.0000	0.00000	0.00000
Total kmol/h	10.0000	39.7131	15.8500	23.8807
Flowrates in kmol/h				
Hydrogen	10.0000	0.0000	0.0000	0.0000
Dichlorosilane	0.0000	0.0000	0.0000	0.0000
Trichlorosilane	0.0000	0.1066	0.0000	0.1066
Silicon TetraCl	0.0000	0.0079	0.0000	7.9241
Hydrogen Chlorid	0.0000	31.6648	0.0000	0.0000
Silicon	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.0176	15.8500	15.8500
Silicon Dioxide	0.0000	7.9162	0.0000	0.0000
Boron Trichlorid	0.0000	0.0000	0.0000	0.0000
Phosphoric Chlor	0.0000	0.0000	0.0000	0.0000

Stream No.	13	14	15	16
Stream Name				
Temp K	572.6719	572.6719	573.0000	572.9728
Pres bar	0.9402	0.9402	1.0000	0.9810
Enth kW	-758.27	-637.60	-400.45	-400.45
Vapor mole fraction	1.0000	0.00000	1.0000	1.0000
Total kmol/h	31.8036	7.9096	5.5650	5.5650
Flowrates in kmol/h				
Hydrogen	0.0000	0.0000	0.0000	0.0000
Dichlorosilane	0.0000	0.0000	0.0000	0.0000
Trichlorosilane	0.1066	0.0000	0.0000	0.0000
Silicon TetraCl	0.0079	0.0000	0.0000	0.0000
Hydrogen Chlorid	31.6648	0.0000	0.0000	0.0000
Silicon	0.0000	0.0000	0.0000	0.0000
Water	0.0176	0.0000	2.9900	2.9900
Silicon Dioxide	0.0066	7.9096	2.5750	2.5750
Boron Trichlorid	0.0000	0.0000	0.0000	0.0000
Phosphoric Chlor	0.0000	0.0000	0.0000	0.0000

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

FLOW SUMMARIES

Stream No.	17	18	19	20
Stream Name				
Temp K	572.9728	509.4411	509.4411	572.6204
Pres bar	0.9810	0.0000	0.0000	0.9402
Enth kW	-2.0713E-028	-755.82	-0.54234	-638.15
Vapor mole fraction	0.00000	1.0000	0.00000	0.00000
Total kmol/h	0.0000	31.7969	0.0066	7.9162
Flowrates in kmol/h				
Hydrogen	0.0000	0.0000	0.0000	0.0000
Dichlorosilane	0.0000	0.0000	0.0000	0.0000
Trichlorosilane	0.0000	0.1066	0.0000	0.0000
Silicon TetraCl	0.0000	0.0079	0.0000	0.0000
Hydrogen Chlorid	0.0000	31.6648	0.0000	0.0000
Silicon	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.0176	0.0000	0.0000
Silicon Dioxide	0.0000	0.0000	0.0066	7.9162
Boron Trichlorid	0.0000	0.0000	0.0000	0.0000
Phosphoric Chlor	0.0000	0.0000	0.0000	0.0000

Stream No.	21	22	23	24
Stream Name				
Temp K	1373.0000	1373.0000	306.8699	329.7928
Pres bar	1.0000	1.0000	1.0000	1.0000
Enth kW	327.46	-1437.9	-513.23	-1179.1
Vapor mole fraction	1.0000	1.0000	0.00000	0.00000
Total kmol/h	30.6257	15.5830	3.3691	6.1696
Flowrates in kmol/h				
Hydrogen	26.5707	0.0000	0.0000	0.0000
Dichlorosilane	0.0000	0.1490	0.1341	0.0000
Trichlorosilane	0.0000	2.5498	2.5495	0.0001
Silicon TetraCl	0.0000	6.8551	0.6855	6.1696
Hydrogen Chlorid	0.0000	6.0292	0.0000	0.0000
Silicon	4.0550	0.0000	0.0000	0.0000
Water	0.0000	0.0000	0.0000	0.0000
Silicon Dioxide	0.0000	0.0000	0.0000	0.0000
Boron Trichlorid	0.0000	0.0000	0.0000	0.0000
Phosphoric Chlor	0.0000	0.0000	0.0000	0.0000

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

FLOW SUMMARIES

Stream No.	29	30	31	32
Stream Name				
Temp K	189.0152	301.2649	307.3381	196.5361
Pres bar	1.0000	1.0000	1.0000	1.0000
Enth kW	-188.52	-8.6615	-1905.1	-713.46
Vapor mole fraction	0.00000	0.00000	0.00000	0.00000
Total kmol/h	6.0443	0.0612	12.5542	9.4134
Flowrates in kmol/h				
Hydrogen	0.0000	0.0000	0.0000	0.0000
Dichlorosilane	0.0149	0.0000	0.0000	0.1490
Trichlorosilane	0.0002	0.0535	10.6565	2.5497
Silicon TetraCl	0.0000	0.0000	1.8900	0.6855
Hydrogen Chlorid	6.0292	0.0000	0.0000	6.0292
Silicon	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.0000	0.0000	0.0000
Silicon Dioxide	0.0000	0.0000	0.0000	0.0000
Boron Trichlorid	0.0000	0.0077	0.0000	0.0000
Phosphoric Chlor	0.0000	0.0000	0.0077	0.0000

Stream No.	33	34	35
Stream Name			
Temp K	270.4577	330.7219	307.1727
Pres bar	1.0000	1.0000	1.0000
Enth kW	-1962.0	-23.338	-1881.8
Vapor mole fraction	0.85347	0.00000	0.00000
Total kmol/h	38.0988	0.1255	12.4287
Flowrates in kmol/h			
Hydrogen	24.4900	0.0000	0.0000
Dichlorosilane	0.1341	0.0000	0.0000
Trichlorosilane	12.7702	0.0001	10.6563
Silicon TetraCl	0.7045	0.1177	1.7723
Hydrogen Chlorid	0.0000	0.0000	0.0000
Silicon	0.0000	0.0000	0.0000
Water	0.0000	0.0000	0.0000
Silicon Dioxide	0.0000	0.0000	0.0000
Boron Trichlorid	0.0000	0.0000	0.0000
Phosphoric Chlor	0.0000	0.0077	0.0000

Job Name: Systems Final Project Impurities   Date: 05/12/2011   Time: 02:29:15

DISTILLATION PROFILE

Unit type : SCDS   Unit name: Eqp # 3

			* Net Flows	*			
	Temp	Pres	Liquid	Vapor	Feeds	Product	Duties
Stg	K	bar	kmol/h	kmol/h	kmol/h	kmol/h	kW
1	304.6	1.00	143.77			10.57	-1087
2	304.7	1.00	143.69	154.33			
3	304.8	1.00	143.55	154.26			
4	305.0	1.00	155.98	154.12	12.43		
5	305.0	1.00	155.97	154.11			
6	305.0	1.00	155.96	154.11			
7	305.0	1.00	155.95	154.10			
8	305.0	1.00	155.96	154.09			
9	305.0	1.00	155.92	154.10			
10	305.0	1.00	155.84	154.06			
11	305.1	1.00	155.65	153.98			
12	305.4	1.00	155.28	153.79			
13	305.9	1.00	154.49	153.42			
14	307.1	1.00	152.89	152.63			
15	309.4	1.00	150.35	151.03			
16	313.1	1.00	147.22	148.48			
17	317.8	1.00	144.64	145.36			
18	322.4	1.00	143.16	142.78			
19	325.7	1.00	142.58	141.30			
20	327.7	1.00		140.72		1.86	1088

Mole Reflux ratio   13.605

Total liquid entering stage   4 at 304.953 K,   155.974 kmol/h.

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

DISTILLATION PROFILE

Unit type : SCDS Unit name: Eqp # 6

			* Net Flows	*			
	Temp	Pres	Liquid	Vapor	Feeds	Product	Duties
Stg	K	bar	kmol/h	kmol/h	kmol/h	kmol/h	kW
1	196.5	1.00	188.27			9.41	-1392
2	284.6	1.00	158.86	197.68			
3	315.3	1.00	172.65	168.27			
4	320.9	1.00	171.44	182.06			
5	324.2	1.00	170.70	180.85			
6	326.2	1.00	170.43	180.11			
7	327.2	1.00	170.34	179.85			
8	327.7	1.00	170.30	179.75			
9	328.0	1.00	170.29	179.72			
10	328.1	1.00	126.47	179.70	15.58		
11	329.5	1.00	127.10	120.30			
12	329.7	1.00	127.11	120.93			
13	329.7	1.00	127.11	120.94			
14	329.8	1.00	127.10	120.94			
15	329.8	1.00	127.10	120.93			
16	329.8	1.00	127.10	120.93			
17	329.8	1.00	127.10	120.93			
18	329.8	1.00	127.10	120.93			
19	329.8	1.00	127.10	120.93			
20	329.8	1.00		120.93		6.17	936.9

Mole Reflux ratio 20.000

Total liquid entering stage 10 at 327.978 K, 170.289 kmol/h.

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

DISTILLATION PROFILE

Unit type : SCDS Unit name: Eqp # 16

Stg	Temp K	Pres bar	* Net Flows * Liquid kmol/h	Vapor kmol/h	Feeds kmol/h	Product kmol/h	Duties kW
1	301.3	1.00	77.13			0.06	-542.3
2	302.7	1.00	77.03	77.19			
3	303.6	1.00	76.98	77.09			
4	304.1	1.00	76.95	77.04			
5	304.3	1.00	76.94	77.01			
6	304.5	1.00	76.93	77.00			
7	304.6	1.00	76.91	76.99			
8	304.6	1.00	76.88	76.97			
9	304.7	1.00	76.81	76.94			
10	305.0	1.00	76.65	76.87			
11	305.4	1.00	62.70	76.71	12.62		
12	305.4	1.00	62.70	50.14			
13	305.4	1.00	62.70	50.14			
14	305.4	1.00	62.70	50.14			
15	305.4	1.00	62.69	50.14			
16	305.5	1.00	62.68	50.14			
17	305.5	1.00	62.64	50.12			
18	305.7	1.00	62.53	50.08			
19	306.1	1.00	62.26	49.98			
20	307.3	1.00		49.71		12.55	354.5

Mole Reflux ratio 1260.283

Total liquid entering stage 11 at 304.952 K, 76.649 kmol/h.

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

DISTILLATION PROFILE

Unit type : SCDS Unit name: Eqp # 17

Stg	Temp K	Pres bar	* Net Flows * Liquid kmol/h	Vapor kmol/h	Feeds kmol/h	Product kmol/h	Duties kW
1	189.0	1.00	30.22			6.04	-165.3
2	195.3	1.00	21.43	36.27			
3	251.5	1.00	17.25	27.48			
4	276.7	1.00	18.44	23.30			
5	282.5	1.00	27.25	24.48	9.41		
6	293.3	1.00	28.08	23.88			
7	297.2	1.00	28.11	24.71			
8	300.6	1.00	28.10	24.74			
9	303.6	1.00	27.96	24.73			
10	306.9	1.00		24.59		3.37	177

Mole Reflux ratio 5.000

Total liquid entering stage 5 at 235.929 K, 24.075 kmol/h.

Job Name: Systems Final Project Impurities Date: 05/12/2011 Time: 02:29:15

DISTILLATION PROFILE

Unit type : SCDS Unit name: Eqp # 19

Stg	Temp K	Pres bar	* Net Flows * Liquid kmol/h	Vapor kmol/h	Feeds kmol/h	Product kmol/h	Duties kW
1	307.2	1.00	1.24			12.43	-98.62
2	309.8	1.00	1.22	13.67			
3	310.2	1.00	1.22	13.65			
4	310.3	1.00	1.21	13.64			
5	310.3	1.00	1.21	13.64			
6	310.3	1.00	1.21	13.64			
7	310.3	1.00	1.21	13.64			
8	310.3	1.00	1.21	13.64			
9	310.3	1.00	1.21	13.64			
10	310.3	1.00	13.51	13.64	12.55		
11	314.5	1.00	13.23	13.38			
12	319.3	1.00	13.02	13.10			
13	323.6	1.00	12.92	12.90			
14	326.5	1.00	12.88	12.79			
15	328.1	1.00	12.87	12.76			
16	329.0	1.00	12.86	12.74			
17	329.4	1.00	12.86	12.74			
18	329.6	1.00	12.86	12.74			
19	329.7	1.00	12.82	12.74			
20	330.7	1.00		12.69		0.13	98.66

Mole Reflux ratio 0.100

Total liquid entering stage 10 at 307.586 K, 13.767 kmol/h.