Modeling, Simulation and Optimization for Decision Making in Chemical Industry

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Abstract In this paper we will model, simulate and identify the optimized parameters for Chlorosilane mixtures. We will simulate two types of feed Hydrogen (H_2), Hydrochloric acid (HCl), Dichlorosilane (SiH_2Cl_2), Trichlorosilane ($SiHCl_3$) and Silicon tetrachloride ($SiCl_4$) as feed compositions.Then we will use Dynamic simulation to do the step test in feed-1 and observe the temperature controllers along with other controllers.

Keywords: Chlorosilane mixtures, Aspen Dynamics, Simulation, Modeling in Chemical Industry

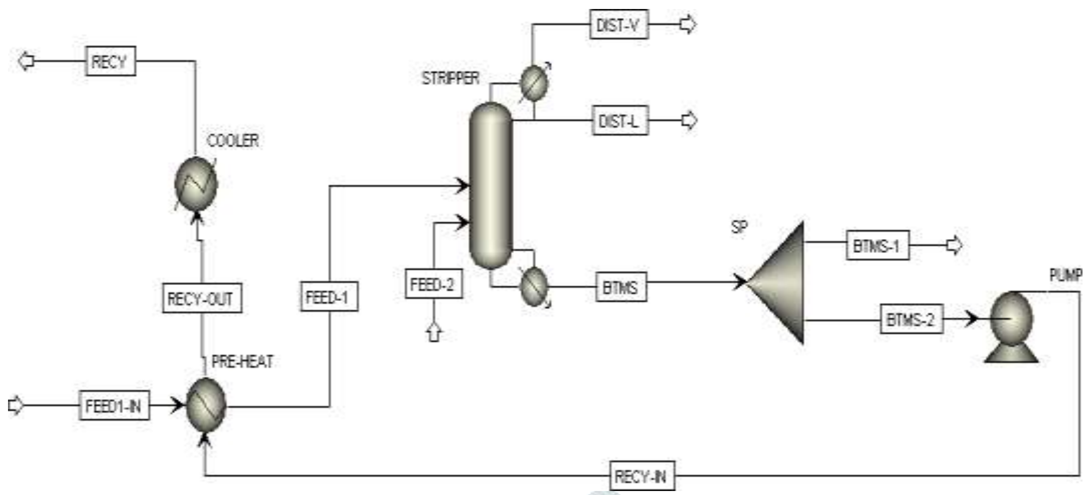
I. Introduction

A stripper is designed to separate Chlorosilane mixtures. Two types of feed are used with Hydrogen (H_2), Hydrochloric acid (HCl), Dichlorosilane (SiH_2Cl_2), Trichlorosilane ($SiHCl_3$) and Silicon tetrachloride ($SiCl_4$) as feed compositions with the following details:

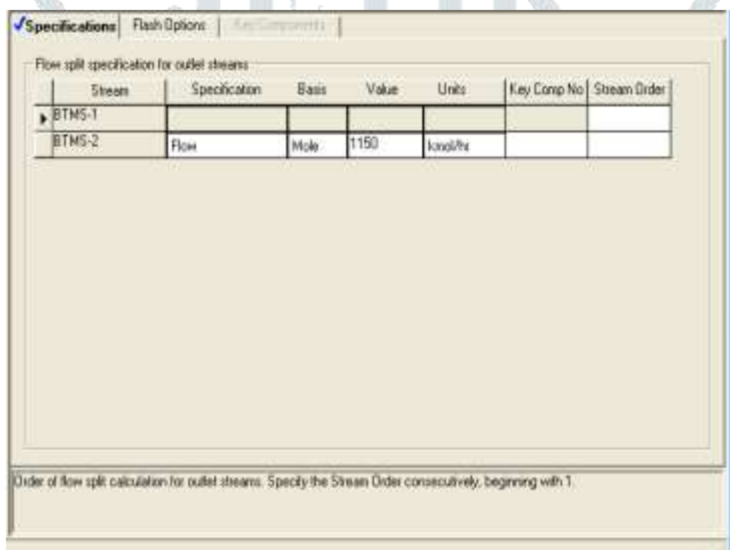
	Flow rate kmole/hr	H_2 (mol %)	HCl (mol %)	SiH_2Cl_2 (mol %)	$SiHCl_3$ (mol %)	$SiCl_4$ (mol %)
Feed 1	1275	0.1	6	4	31	58.9
Feed 2	460	100 ppm	0.5	3	29.49	67

Feed-1 is initially at 15.8 barg and -53 ^{O}C which is pre-heated using a recycled stream to 7.4 ^{O}C, fed into stripper along with feed-2 to separate H_2 and HCl from the Chlorosilanes. H_2 and HCl contents in the chlorosilanes must be below 0.01 ppb by mole and the chlorosilane loss must be below 0.8 kg/hr. Stripper is simulated using the given information with 66 stages including condenser and reboiler, with optimum feed tray as 29th stage with tower diameter as 1 m on the top and 3.7 m for the bottom section. Stripper is designed using bottoms to feed ratio of 0.95382075 and the reflux ratio as 0.9841. Dynamic simulation is used to do the step test in feed-1 and observe the temperature controllers along with other controllers. Bottoms stream is separated using splitter with 1150 kmol/hr of stream entering the pump as BTMS-2 and the other stream as BTMS-1. BTMS-2 stream is taken through pump, with discharge pressure of 8.8 bars and pre-heater to heat the FEED1-IN stream from -53 to 7.3 ^{O}C and finally sent to the cooler to be recycled at -60 ^{O}C.

Process Flow Diagram:



Specification for splitter:

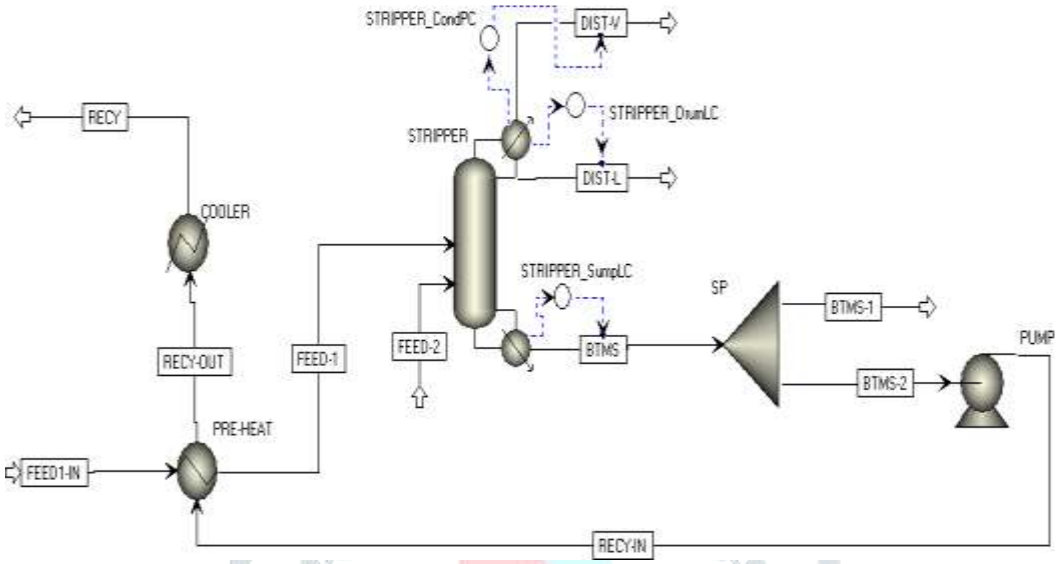


II. Simulation Methods:

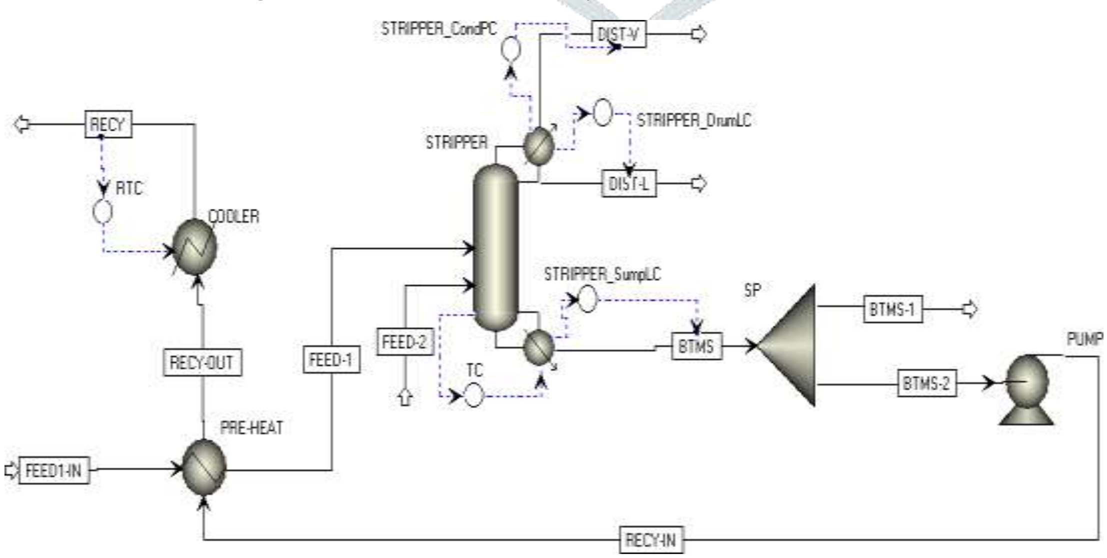
Since the number of equilibrium stages, reflux ratio, bottoms to feed ratio and the feed tray are given, stripper is simulated using the rigorous column directly. NRTL property method is used for the simulation and the results are checked for the given specifications, if the results do not meet the specified results, stripper parameters such as reflux ratio, distillate to feed ratio, bottoms to feed ratio, distillate flow rate and bottoms flow rate should be varied.

Procedure:

The process is simulated using the given conditions in steady state and the results are noted. In order to run the process in dynamic simulation, steady state process should be imported from ASPEN Plus to ASPEN Dynamics. Also to proceed in dynamic simulation, the length and diameter of the reflux drum are given as 2.15 m and 1.4 m respectively with vertical and elliptical geometry; height and diameter of the sump are 0.25 m and 3.7 m respectively with hemispherical geometry with liquid fraction of 0.7 in both sump and drum. Also the weir heights are 5.2 cm for top section and 5.7 cm for bottom section with tray spacing of 35 cm. Now the file is ready to export for dynamic simulation and initially the process flow diagram in dynamics state will be as shown below with column pressure controller, drum and level controllers.



In the above dynamic flow diagram, pressure controller for the condenser, level controllers for reboiler and reflux drum are assigned in the flow driven dynamic simulation. For this column a temperature controller (TC) is set with 10^{th} stage temperature as process variable and its out put connected to the reboiler heat duty. Also another temperature controller (RTC) is set for RECY stream, with its temperature as process variable and COOLER duty as out put of the controller and these two controllers should be in reverse acting. As the process variable of two temperature controller increases, its output decreases so these should be in reverse action where as for the pressure and two level controllers output increases as process variable increases so these controllers will be in direct action. The flow diagram with these changes in the controller set up is shown below:



III. Simulation Results:

The steady state simulation results for the stripper are shown below:

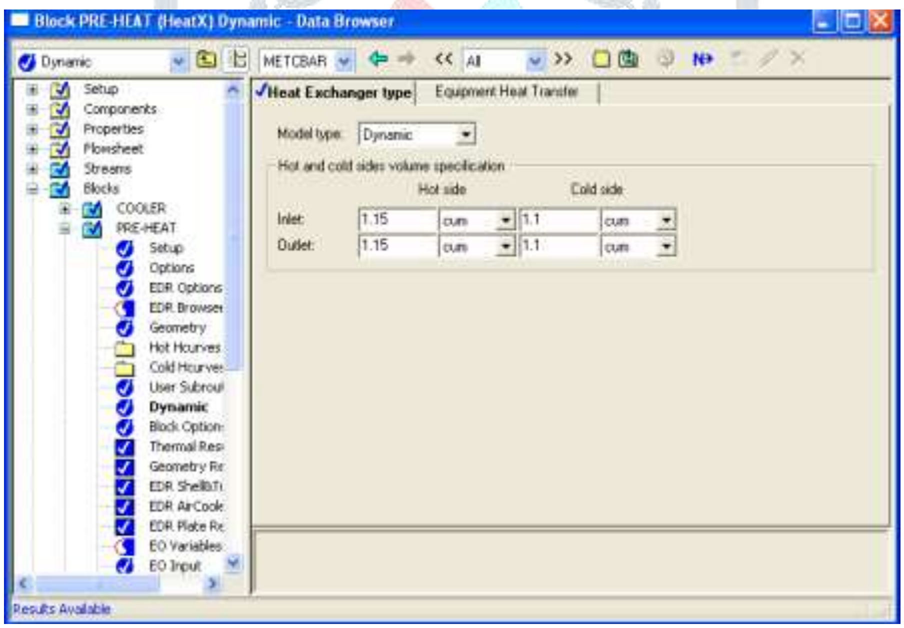
These results meet the specified parameters as mentioned in the problem, so with these result, the dynamic simulation of the column is preceded by inputting the dynamic data of the column.

	FEED-2	FEED-1	DIST-L	DIST-V	BTMS	RECY-IN	RECY
	STRIPPER	STRIPPER			SP	PRE-HEAT	
		PRE-HEAT	STRIPPER	STRIPPER	STRIPPER	PUMP	COOLER
	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED							
Mole Flow kmol/hr							
H2	0.046	1.275	4.28E-03	1.316716	1.65E-33	1.15E-33	1.15E-33
HCL	2.3	76.5	69.70107	9.098929	1.20E-27	8.35E-28	8.35E-28
SIH2CL2	13.8	51	4.84E-07	7.66E-10	64.8	45.03048	45.03048
SIHCL3	135.654	395.25	3.57E-17	1.77E-20	530.904	368.9331	368.9331
SICL4	308.2	750.975	1.00E-24	1.24E-28	1059.175	736.0364	736.0364
Mole Frac							
H2	1.00E-04	1.00E-03	6.15E-05	0.126417	**1.00E-36**	1.00E-36	1.00E-36
HCL	5.00E-03	0.06	0.999939	0.873583	**7.26E-31**	7.26E-31	7.26E-31
SIH2CL2	0.03	0.04	6.95E-09	7.35E-11	0.039157	0.039157	0.039157
SIHCL3	0.2949	0.31	5.12E-19	1.70E-21	0.320811	0.320811	0.320811
SICL4	0.67	0.589	1.44E-26	1.19E-29	0.640032	0.640032	0.640032
Mass Flow kg/hr							
H2	0.09273	2.570247	8.64E-03	2.654341	3.34E-33	2.32E-33	2.32E-33
HCL	83.85947	2789.239	2541.346	331.7528	4.38E-26	3.04E-26	3.04E-26
SIH2CL2	1393.894	5151.346	**4.89E-05**	7.73E-08	6545.239	4548.384	4548.384
SIHCL3	18374.54	53537.22	**4.84E-15**	2.40E-18	71911.76	49972.55	49972.55
SICL4	52362.04	1.28E+05	**1.70E-22**	2.11E-26	1.80E+05	1.25E+05	1.25E+05
Mass Frac							
H2	1.28E-06	1.36E-05	3.40E-06	7.94E-03	1.29E-38	1.29E-38	1.29E-38
HCL	1.16E-03	0.014753	0.999997	0.992063	1.69E-31	1.69E-31	1.69E-31
SIH2CL2	0.019302	0.027246	1.92E-08	2.31E-10	0.025329	0.025329	0.025329
SIHCL3	0.254444	0.283164	1.90E-18	7.16E-21	0.278289	0.278289	0.278289
SICL4	0.725091	0.674824	6.71E-26	6.31E-29	0.696382	0.696382	0.696382
Total Flow kmol/hr	460	1275	69.70536	10.41564	1654.879	1150	1150
Total Flow kg/hr	72214.43	1.89E+05	2541.354	334.4071	2.58E+05	1.80E+05	1.80E+05
Total Flow cum/hr	49.47924	130.8124	2.360796	28.05515	219.7197	152.6862	113.6947
Temperature C	7.4	7.4	-45.9447	-45.9447	128.2036	128.2029	-60
Pressure bar	15.8	16.81325	7.01325	7.01325	8.81325	8.8	5.02E-03
Vapor Frac	0	0	0	1	0	0	0
Liquid Frac	1	1	1	0	1	1	1

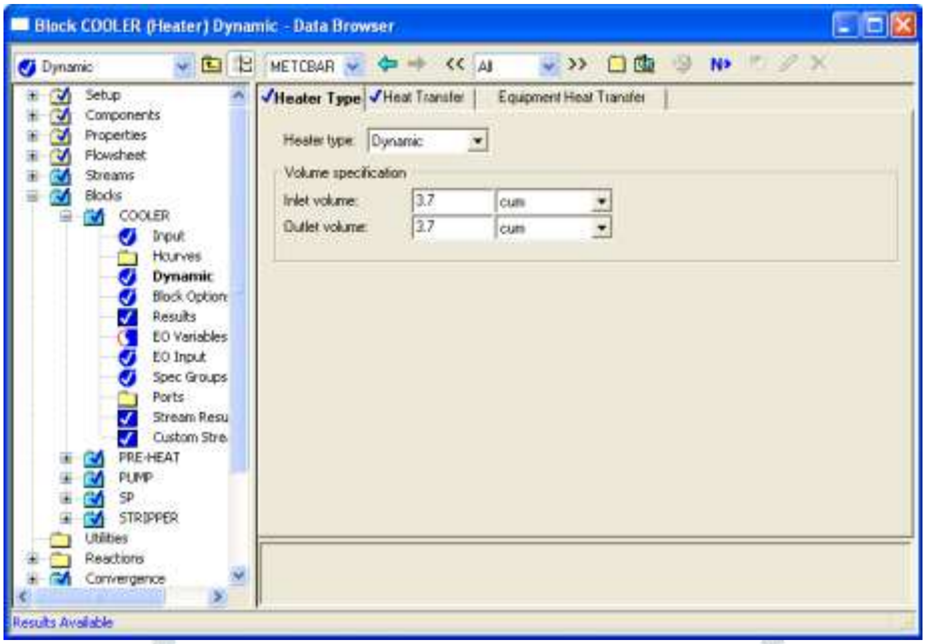
Solid Frac	0	0	0	0	0	0	0
Enthalpy kcal/mol	-150.819	-141.462	-26.0172	-19.7531	-145.298	-145.298	-151.771
Enthalpy kcal/kg	-960.706	-953.964	-713.61	-615.241	-930.51	-930.511	-971.967
Enthalpy Gcal/hr	-69.3768	-180.364	-1.81354	-0.20574	-240.45	-167.093	-174.537
Entropy cal/mol-K	-51.1551	-48.1789	-18.3723	-2.88182	-38.4589	-38.459	-59.4445
Entropy cal/gm-K	-0.32585	-0.3249	-0.50392	-0.08976	-0.2463	-0.2463	-0.38069
Density kmol/cum	9.296829	9.746784	29.52621	0.371256	7.531773	7.531786	10.11481
Density kg/cum	1459.49	1445.339	1076.482	11.91964	1176.075	1176.077	1579.412
Average MW	156.9879	148.2888	36.45852	32.10623	156.1485	156.1485	156.1485
Liq Vol 60F cum/hr	50.67306	135.3568	3.733266	0.557839	181.7388	126.293	126.293

In dynamic state, results are checked by changing the shell side and tube side to hot and cold fluids. It's observed that the results are same in either case, so dynamics is preceded for pre-heater with hot fluid on shell side and cold fluid on tube side. Also for cooler cold fluid is taken on tube side.

Pre-heater specifications:



Cooler Specifications:

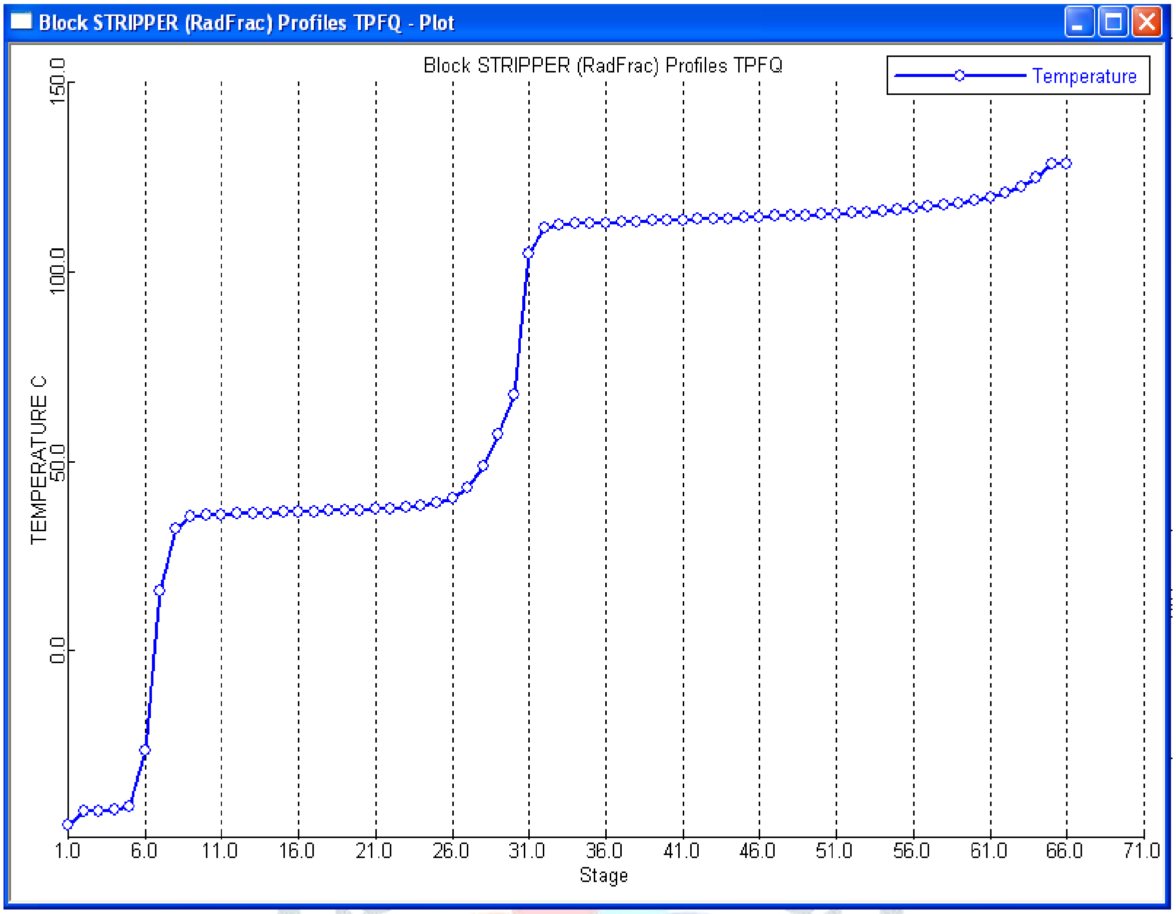


Stream results with Dynamic input for stripper, pre-heater and cooler:

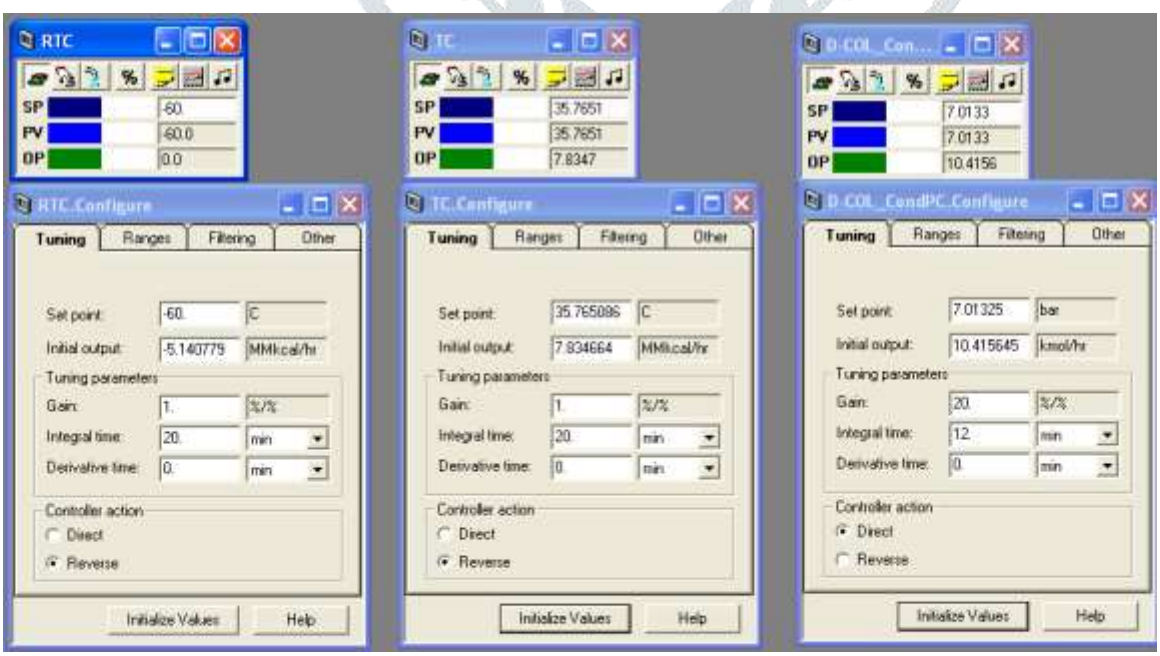
	FEED-2	FEED1-IN	DIST-L	DIST-V	BTMS	RECY-IN	RECY
	STRIPPER	PRE-HEAT			SP	PRE-HEAT	
			STRIPPER	STRIPPER	STRIPPER	PUMP	COOLER
	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED							
Mole Flow kmol/hr							
H2	0.046	1.275	4.28E-03	1.316716	1.65E-33	1.15E-33	1.15E-33
HCL	2.3	76.5	69.70107	9.098929	1.20E-27	8.35E-28	8.35E-28
SIH2CL2	13.8	51	4.84E-07	7.66E-10	64.8	45.03048	45.0304 8
SIHCL3	135.654	395.25	3.57E-17	1.77E-20	530.904	368.9331	368.933 1
SICL4	308.2	750.975	1.00E-24	1.24E-28	1059.175	736.0364	736.036 4
Mole Frac							
H2	1.00E-04	1.00E-03	6.15E-05	0.126417	**1.00E-36**	1.00E-36	1.00E-36
HCL	5.00E-03	0.06	0.999939	0.873583	**7.26E-31**	7.26E-31	7.26E-31
SIH2CL2	0.03	0.04	6.95E-09	7.35E-11	0.039157	0.039157	0.03915 7
SIHCL3	0.2949	0.31	5.12E-19	1.70E-21	0.320811	0.320811	0.32081 1
SICL4	0.67	0.589	1.44E-26	1.19E-29	0.640032	0.640032	0.64003 2
Mass Flow kg/hr							
H2	0.09273	2.570247	8.64E-03	2.654341	3.34E-33	2.32E-33	2.32E-33
HCL	83.85947	2789.239	2541.346	331.7528	4.38E-26	3.04E-26	3.04E-26

SIH2CL2	1393.894	5151.346	**4.89E-05**	7.73E-08	6545.239	4548.384	4548.384
SIHCL3	18374.54	53537.22	**4.84E-15**	2.40E-18	71911.76	49972.55	49972.55
SICL4	52362.04	1.28E+05	**1.70E-22**	2.11E-26	1.80E+05	1.25E+05	1.25E+05
Mass Frac							
H2	1.28E-06	1.36E-05	3.40E-06	7.94E-03	1.29E-38	1.29E-38	1.29E-38
HCL	1.16E-03	0.014753	0.999997	0.992063	1.69E-31	1.69E-31	1.69E-31
SIH2CL2	0.019302	0.027246	1.92E-08	2.31E-10	0.025329	0.025329	0.025329
SIHCL3	0.254444	0.283164	1.90E-18	7.16E-21	0.278289	0.278289	0.278289
SICL4	0.725091	0.674824	6.71E-26	6.31E-29	0.696382	0.696382	0.69638
							2
Total Flow kmol/hr	460	1275	69.70536	10.41564	1654.879	1150	1150
Total Flow kg/hr	72214.43	1.89E+05	2541.354	334.4071	2.58E+05	1.80E+05	1.80E+05
Total Flow cum/hr	49.47924	121.2706	2.360796	28.05515	219.7197	152.6862	113.6947
Temperature C	7.4	-53	-45.9447	-45.9447	128.2036	128.2029	-60
Pressure bar	15.8	16.81325	7.01325	7.01325	8.81325	8.8	5.02E-03
Vapor Frac	0	0	0	1	0	0	0
Liquid Frac	1	1	1	0	1	1	1
Solid Frac	0	0	0	0	0	0	0
Enthalpy kcal/mol	-150.819	-143.269	-26.0172	-19.7531	-145.298	-145.298	-151.771
Enthalpy kcal/kg	-960.706	-966.149	-713.61	-615.241	-930.51	-930.511	-971.967
Enthalpy Gcal/hr	-69.3768	-182.668	-1.81354	-0.20574	-240.45	-167.093	-174.537
Entropy cal/mol-K	-51.1551	-55.4737	-18.3723	-2.88182	-38.4589	-38.459	-59.4445
Entropy cal/gm-K	-0.32585	-0.37409	-0.50392	-0.08976	-0.2463	-0.2463	-0.38069
Density kmol/cum	9.296829	10.51368	29.52621	0.371256	7.531773	7.531786	10.11481
Density kg/cum	1459.49	1559.061	1076.482	11.91964	1176.075	1176.077	1579.412
Average MW	156.9879	148.2888	36.45852	32.10623	156.1485	156.1485	156.1485
Liq Vol 60F cum/hr	50.67306	135.3568	3.733266	0.557839	181.7388	126.293	126.293

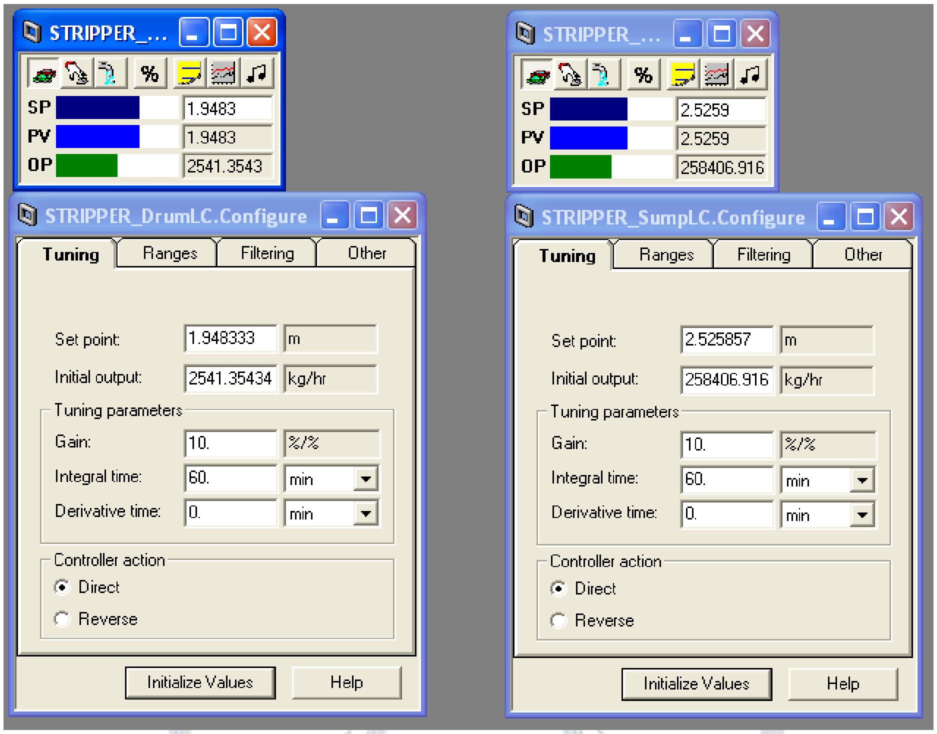
The temperature profile of the column is shown below with number of stages (n) on X-axis and temperature in ^oC on Y-axis;



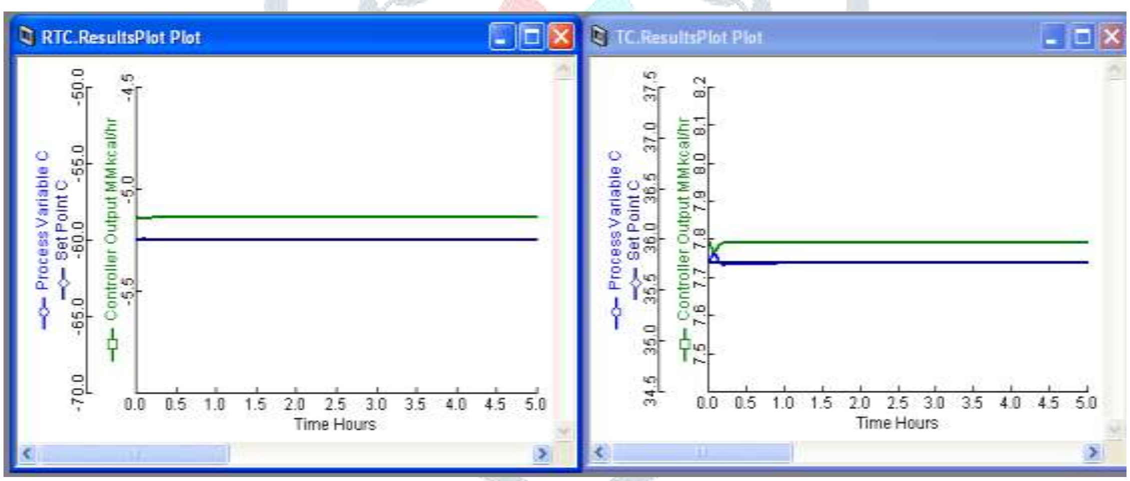
For the temperature controller,controller action is taken as reverse because; as the temperature of the stage increases the reboiler duty decreases. Also for recycle temperature controller as the temperature of recycle stream increases, cooling duty of the cooler decreases. Pressure controller is in direct action and the initial controller settings are shown below:



The two level controller settings are shown below, both in direct action

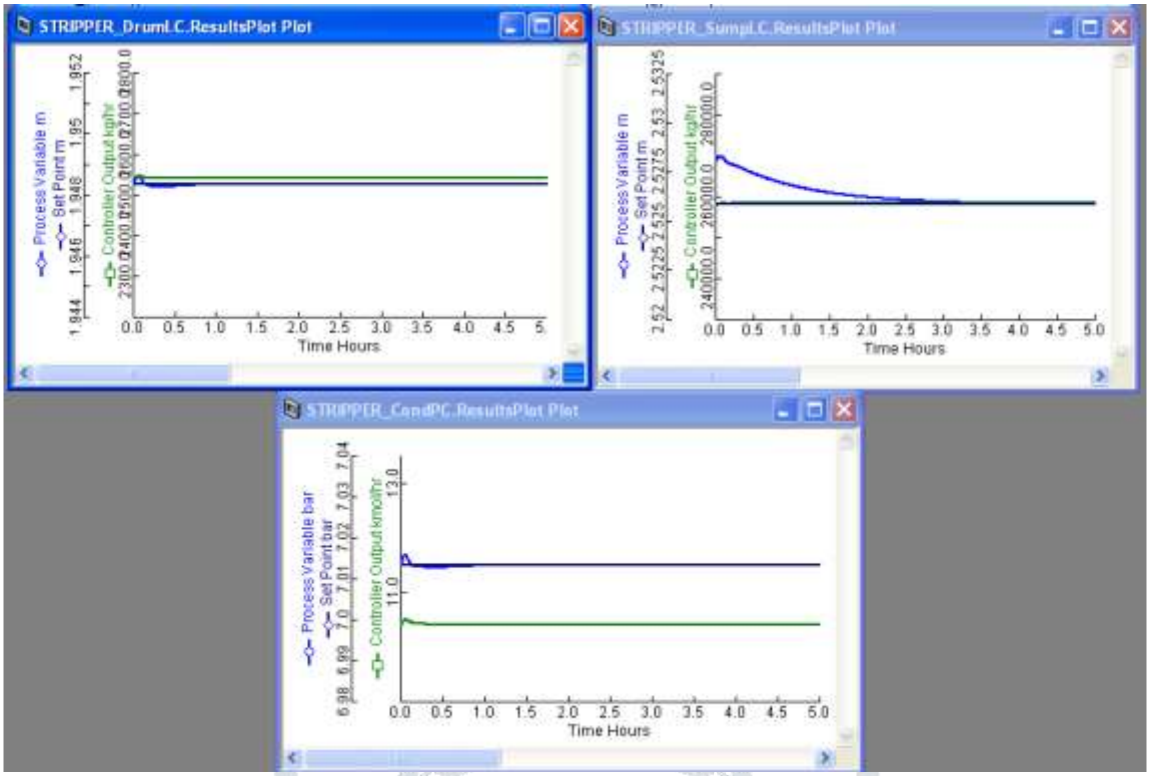


The initial response of two temperature controllers are shown below:



In the above plots, it is observed that both the controllers are in steady state when there is no disturbance and it takes very less time to reach steady state.

The initial response of pressure, sump and level controllers are shown below:



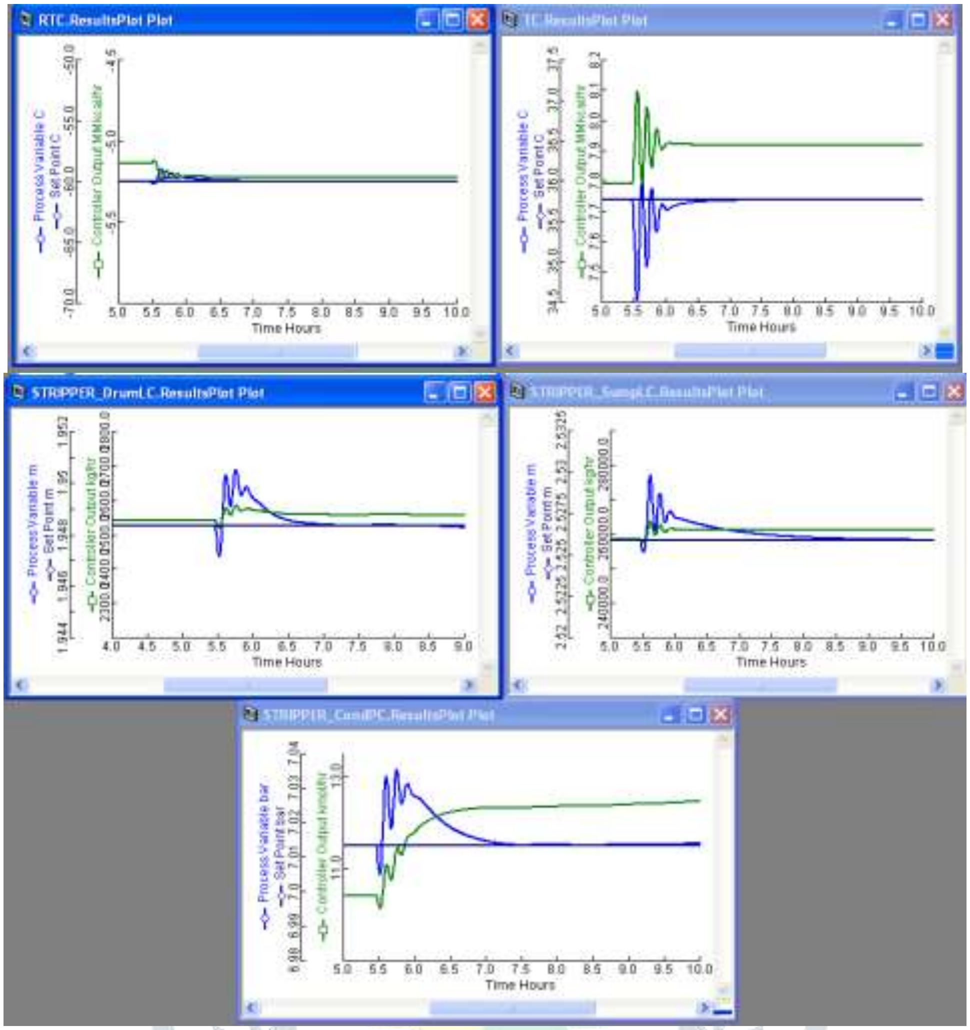
In the above plots, sump level decreases steadily from its initial value to reach steady state, where as the drum and pressure cotrollers have very small decrease in their values to reach steady state.

For these controllers, step test is made by varying the FEED-IN flow rate and the responses of the controllers are obseerved. Fisrt step test is made from 1275 ro 1295 kmol/hr and the responses are shown below:

FEED1-IN.Manipulate Table

	Description	Value	Units	Spec
FR	Specified total molar flow	1295.0	kmol/hr	Fixed
FmR	Specified total mass flow	192034.0	kg/hr	Free
FvR	Specified total volume flow	123.173	m3/hr	Free
T	Temperature	-53.0	C	Fixed
P	Pressure	16.8132	bar	Fixed
vfR	Specified molar vapor fraction	-0.124894		Free
ZR(*)				
ZR("H2")	Specified mole fraction	1.e-003	kmol/kmol	Fixed
ZR("HCL")	Specified mole fraction	0.06	kmol/kmol	Fixed
ZR("SICL4")	Specified mole fraction	0.589	kmol/kmol	Fixed
ZR("SIH2CL2")	Specified mole fraction	0.04	kmol/kmol	Fixed
ZR("SIHCL3")	Specified mole fraction	0.31	kmol/kmol	Fixed

Responses of the controller are shown below:



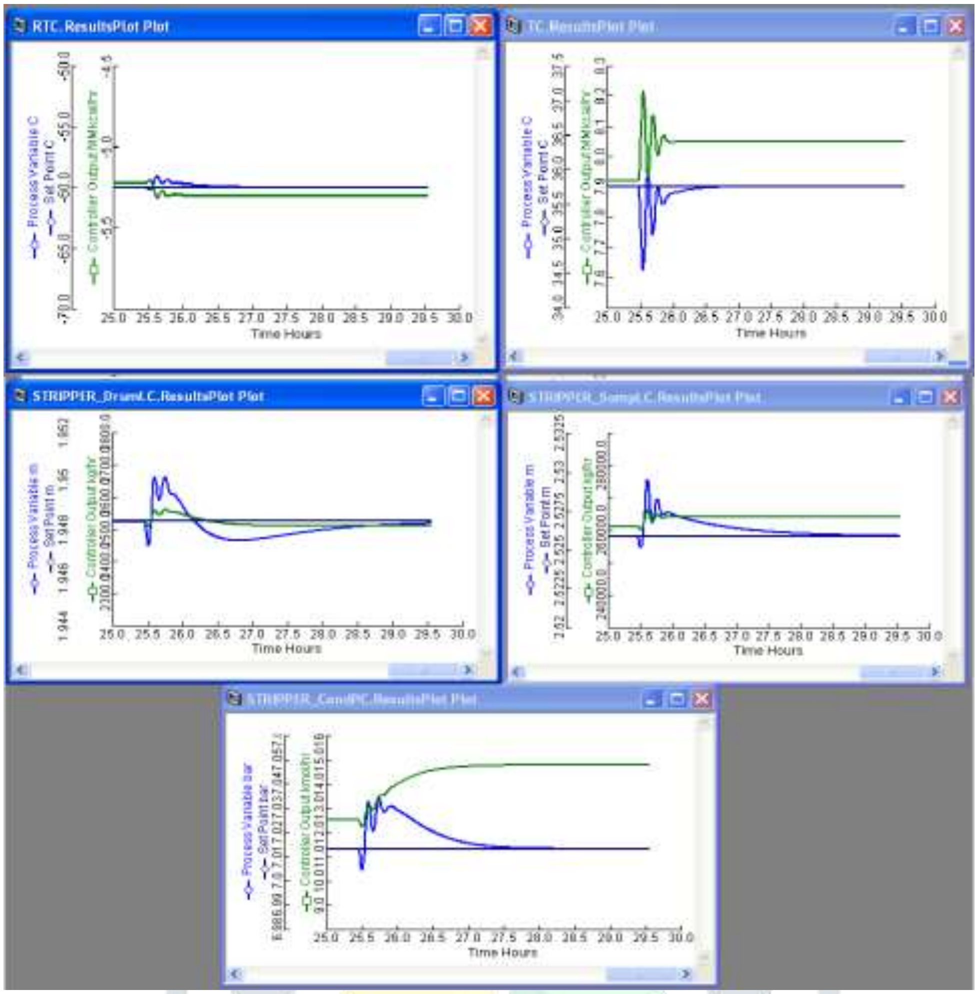
From the above response it is observed that in recycle temperature controller, temperature of the recycle stream varies suddenly and then reaches steady state. It increases gradually and slowly reaches steady state because of sudden increase in feed flow. Because of increase in feed flow, column reboiler duty increases along with drum and sump levels as the pressure also increases. But all other controllers fisrt decreases with step uop change and increases slowly and reaches steady state.

Step up test from 1295 to 1315 kmol/hr:

FEED1-IN.Manipulate Table

	Description	Value	Units	Spec
FR	Specified total molar flow	1315.0	kmol/hr	Fixed
FmR	Specified total mass flow	192034.0	kg/hr	Free
FvR	Specified total volume flow	123.173	m3/hr	Free
T	Temperature	-53.0	C	Fixed
P	Pressure	16.8132	bar	Fixed
vfR	Specified molar vapor fraction	-0.124894		Free
ZR("")				
ZR("H2")	Specified mole fraction	1.e-003	kmol/kmol	Fixed
ZR("HCL")	Specified mole fraction	0.06	kmol/kmol	Fixed
ZR("SICL4")	Specified mole fraction	0.589	kmol/kmol	Fixed
ZR("SIH2CL2")	Specified mole fraction	0.04	kmol/kmol	Fixed
ZR("SIHCL3")	Specified mole fraction	0.31	kmol/kmol	Fixed

Responses of the controller are shown below:



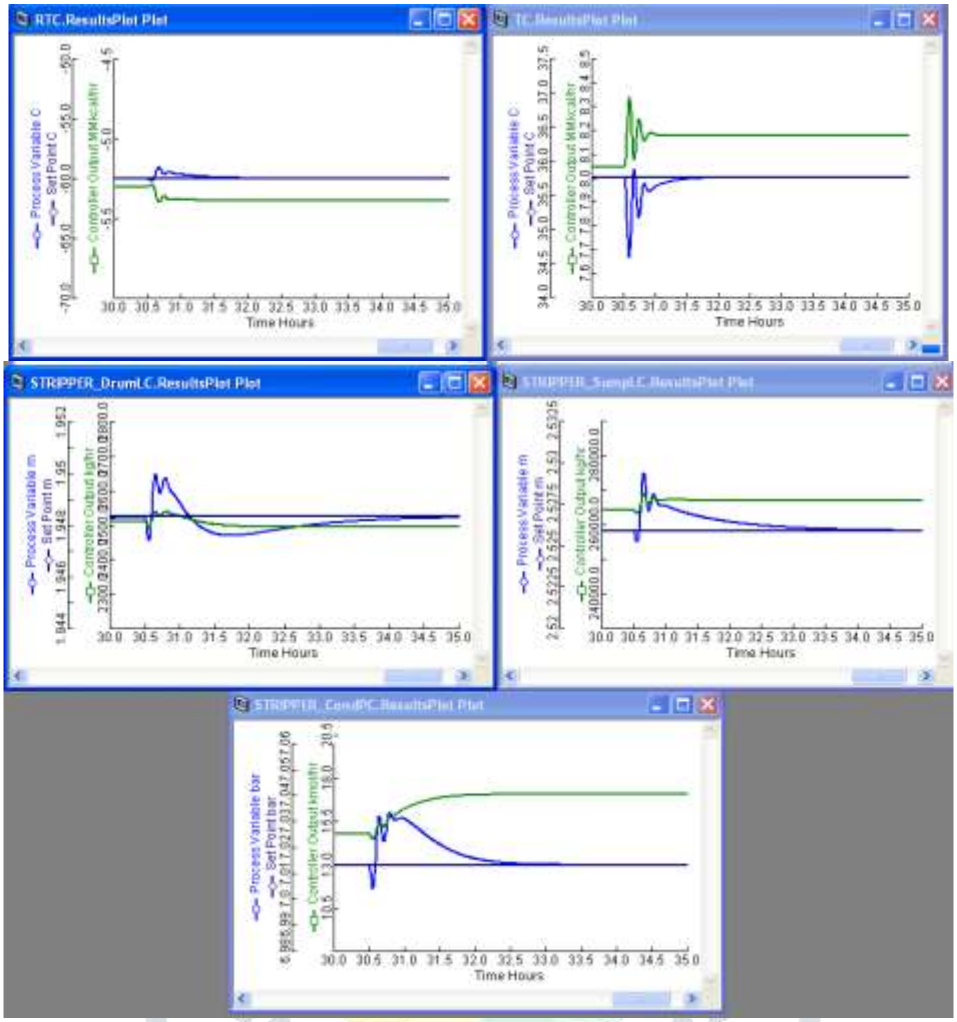
From the above plot, its clear that after reaching the steady state with a disturbance initially, controllers responds fast and takes less time to reach steady state in order to compensate the disturbance. The responses are similar to the previous steu change but with quicker action to reach steady state.

Step up change from 1315 to 1335 kmol/hr

FEED1-IN.Manipulate Table

	Description	Value	Units	Spec
FR	Specified total molar flow	1335.0	kmol/hr	Fixed
FmR	Specified total mass flow	195000.0	kg/hr	Free
FvR	Specified total volume flow	125.075	m3/hr	Free
T	Temperature	-53.0	C	Fixed
P	Pressure	16.8132	bar	Fixed
vfR	Specified molar vapor fraction	-0.124894		Free
ZR("*")				
ZR("H2")	Specified mole fraction	1.e-003	kmol/kmol	Fixed
ZR("HCL")	Specified mole fraction	0.06	kmol/kmol	Fixed
ZR("SICL4")	Specified mole fraction	0.589	kmol/kmol	Fixed
ZR("SIH2CL2")	Specified mole fraction	0.04	kmol/kmol	Fixed
ZR("SIHCL3")	Specified mole fraction	0.31	kmol/kmol	Fixed

Controller response for the above step change:

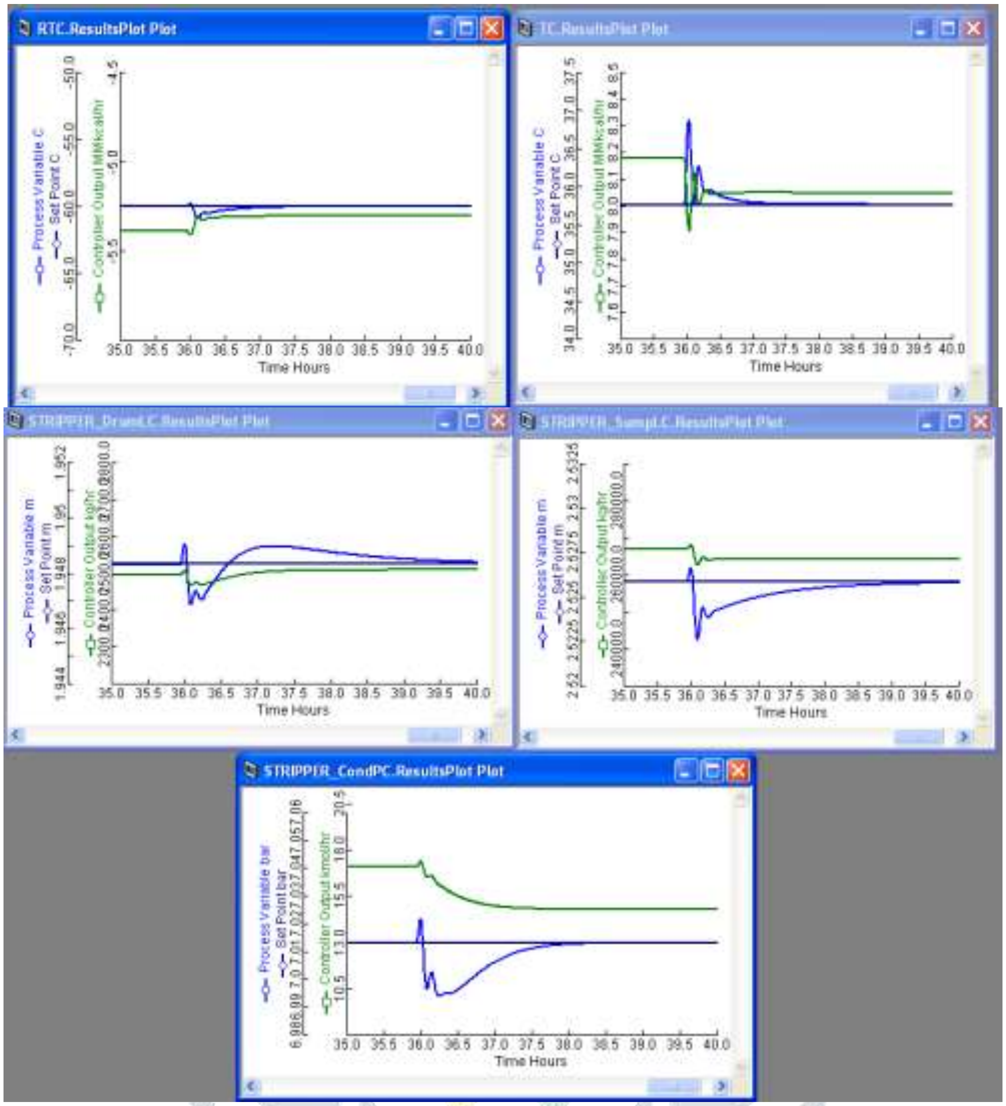


Step down test from 1335 to 1315 kmol/hr

FEED1-IN.Manipulate Table

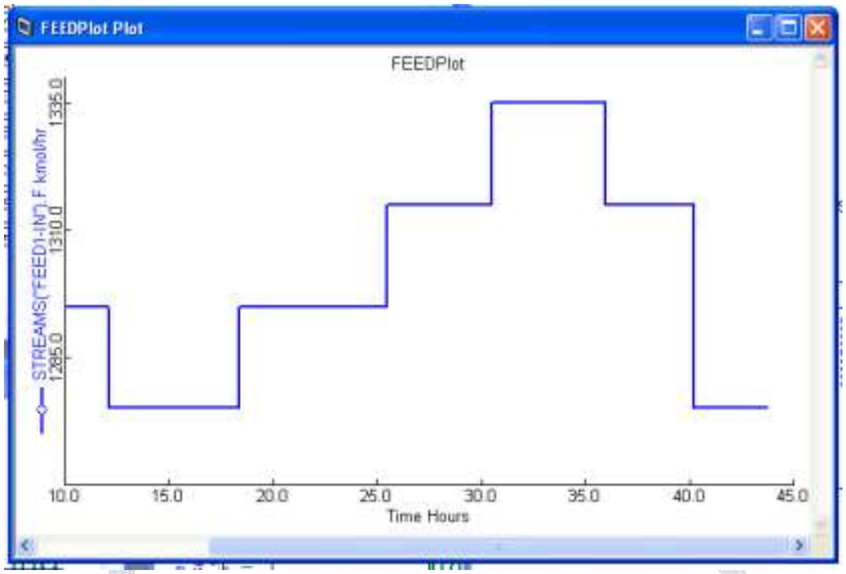
	Description	Value	Units	Spec
FR	Specified total molar flow	1315.0	kmol/hr	Fixed
FmR	Specified total mass flow	197966.0	kg/hr	Free
FvR	Specified total volume flow	126.977	m3/hr	Free
T	Temperature	-53.0	C	Fixed
P	Pressure	16.8132	bar	Fixed
vfR	Specified molar vapor fraction	-0.124894		Free
ZR(*)				
ZR("H2")	Specified mole fraction	1.e-003	kmol/kmol	Fixed
ZR("HCL")	Specified mole fraction	0.06	kmol/kmol	Fixed
ZR("SICL4")	Specified mole fraction	0.589	kmol/kmol	Fixed
ZR("SIH2CL2")	Specified mole fraction	0.04	kmol/kmol	Fixed
ZR("SIHCL3")	Specified mole fraction	0.31	kmol/kmol	Fixed

Response of controllers



From the above, it is evident that controllers reach steady state slowly in order to over come the disturbance. Also because of decrease in feed we can see that recycle temperature controllerdecreases there by increasing the cooling duty of cooler and reaches steady state but in the column temperature controller, reboiler duty decreases suddenly and reaches a value less than the previous steady state valu. And the two level controllers decrase suddenly and then increases slowly to reach steady state.

The change in feed flow is plotted for the given step changes:



IV. Conclusion

Hence the distillation controls of a chlorosilane mixture is set up using Aspen Dynamics with the given data in the problem according to the required specifications and a temperature controller is set up with 10th stage temperature as process variable and the output is connected to the reboiler duty, and the recycle temperature controller is set up to observe the changes in the recycle stream temperature when a step change is given.

Few step-up changes and one step down change is made in the feed mole flow and the controller responses are observed, the corresponding temperature changes records to achieve optimized environment in chlorosilane chemical plant.