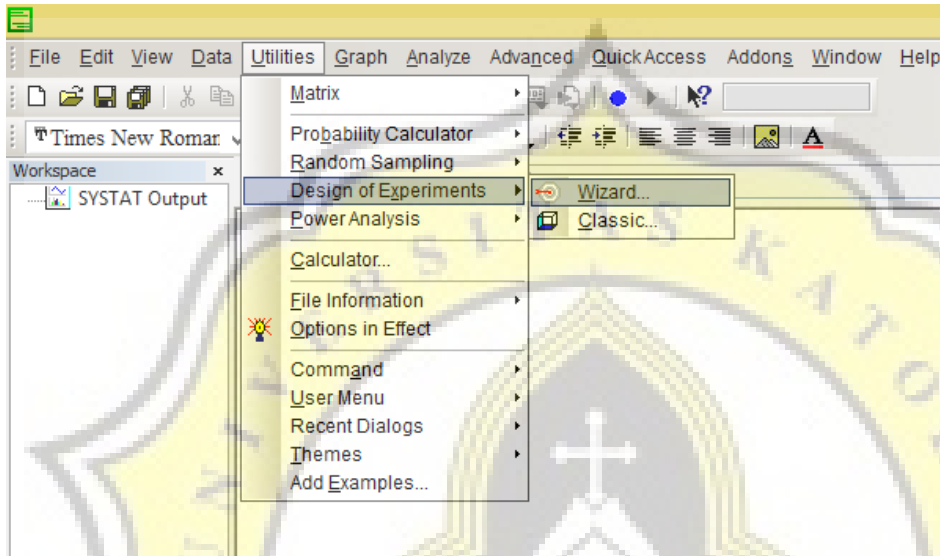


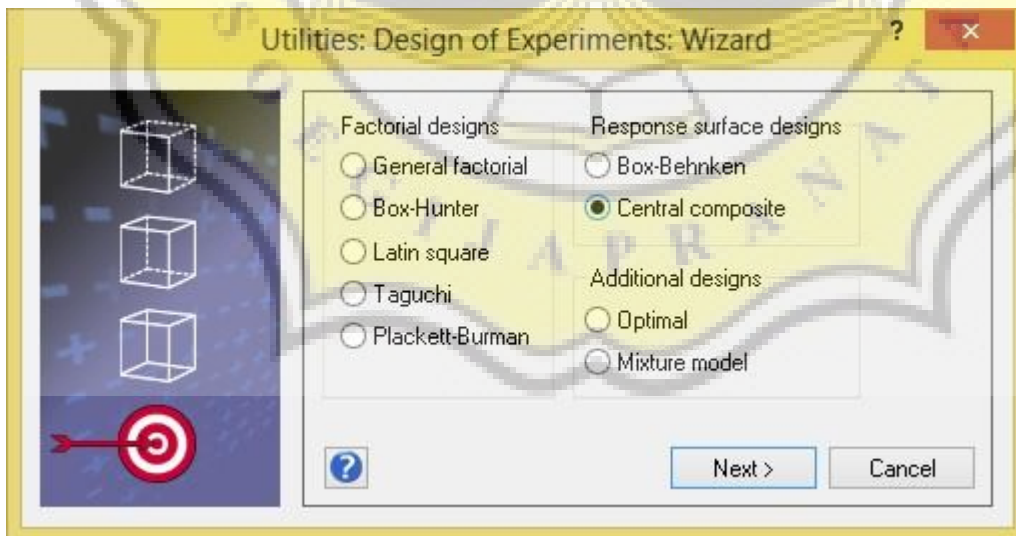
7. APPENDICES

7.1. Determining Experimental Design by Using Design of Experiments Wizard

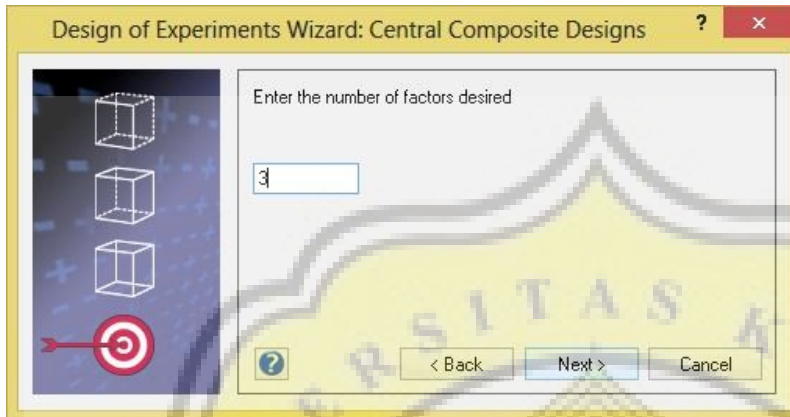
1) By using SYSTAT 12.0, click “**Utilities > Design of Experiments > Wizard**” and continue with the step-by-step guide as shown in figures below.



2) Then, a dialog box “Utilities: Design of Experiments: Wizard” will appear, and choose “**Central composite**” in Response surface designs submenu. Then, click **Next**.



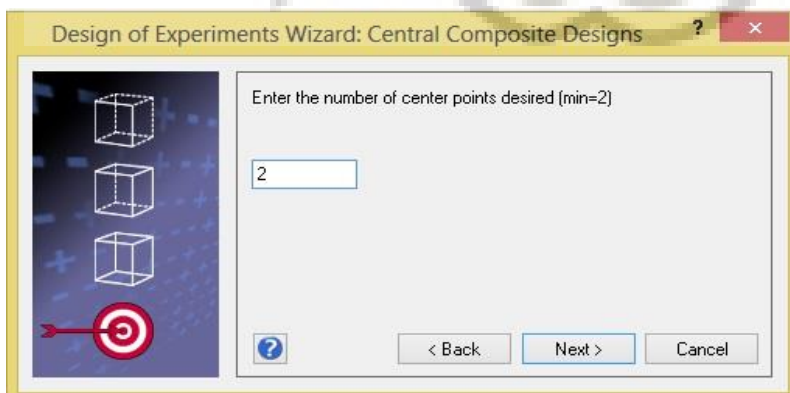
3) Then, you will be asked to enter the number of factors desired. Since the number of factors used in this experiment were three (3), then the answer box should be filled by “3”. Then, click **Next**



4) Choose “No” for the the next question, then click **Next**

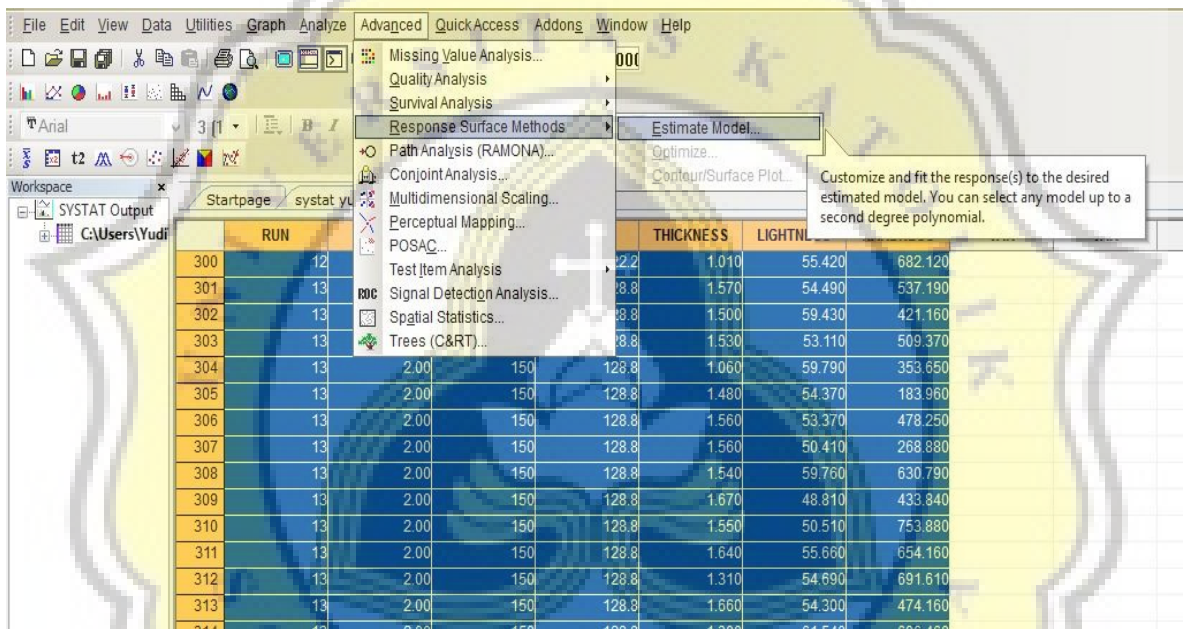


5) For the last step, you will be asked to enter the number of center points desired. In this experiment, two center points were used, so number “2” was filled in the blank. Then, click **Next**

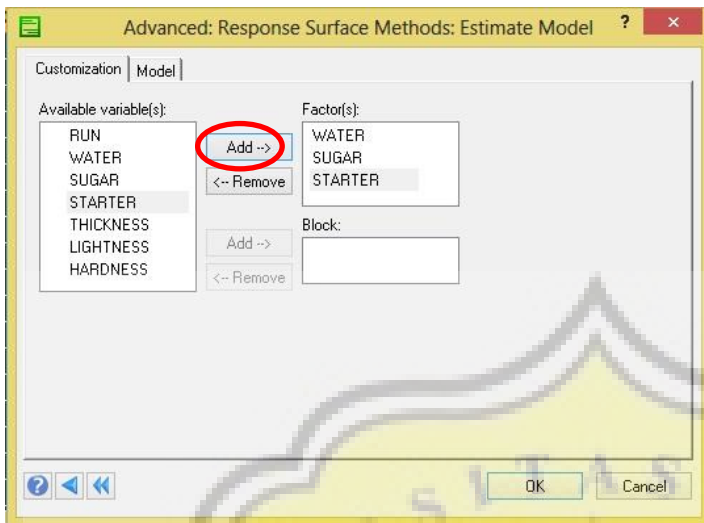


7.2. Model Estimation for the Results by Response Surface Methods

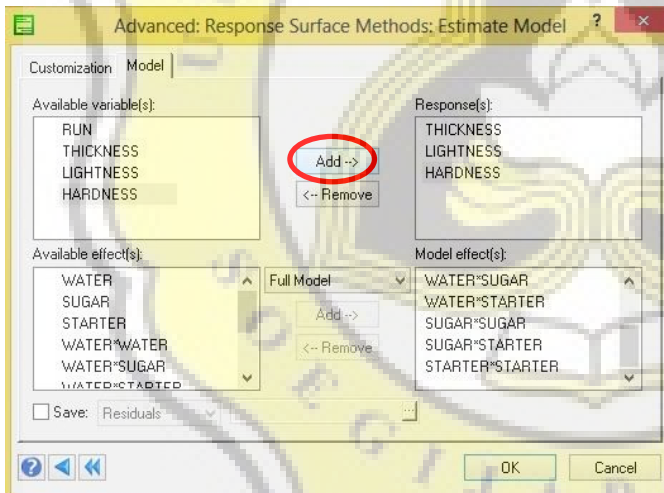
1) First of all, each result should be placed into the SYSTAT Data cells, with the subclass of Run, Water (X1), Sugar (X2), and Starter (X3), Thickness, Lightness, and Hardness. As there were 16 runs, and 25 replication for each runs, there will be 400 rows of data. After the data is placed in the cells and blocked, click “**Advanced > Response Surface Methods > Estimate Model**”



2) Then, a dialog box will appear. In customization tab, variables used in this experiment were added into Factor(s) box by clicking the factors in the Available variable(s) box and then click Add button.

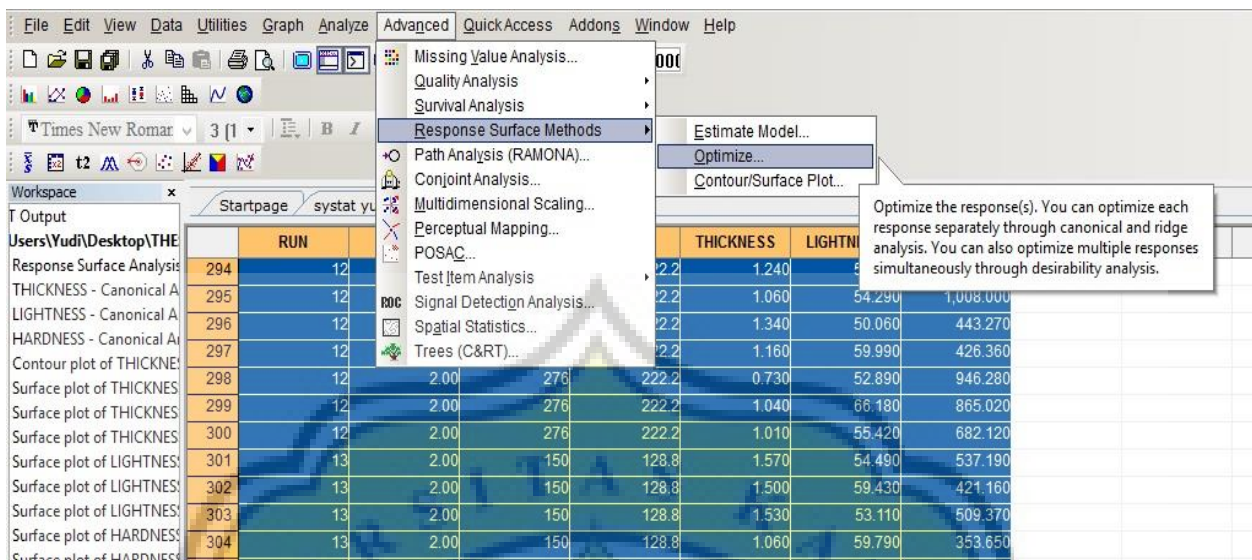


3) In the Model tab, parameters used in this experiment were added into Response(s) box by clicking the factors in the Available variable(s) box and then click Add button. Then, click **OK**

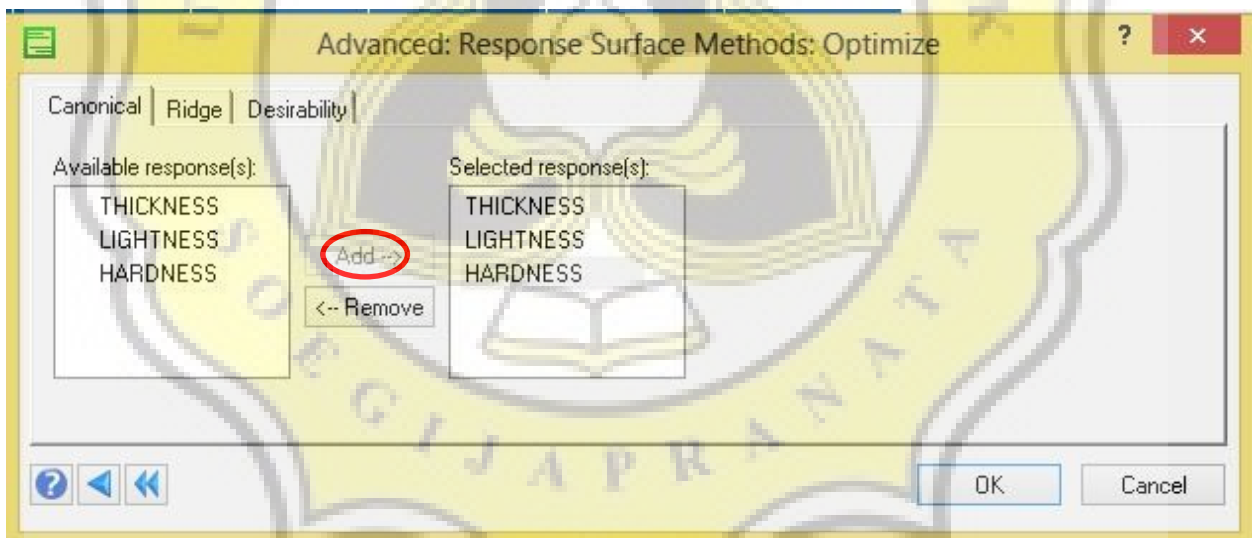


7.3. Canonical Analysis

1) After finishing Model Estimation in Response Surface Methods (RSM), an optimization by using canonical analysis is needed. In order to do this, block all the data, and then click **“Advanced > Response Surface Methods > Optimize”**



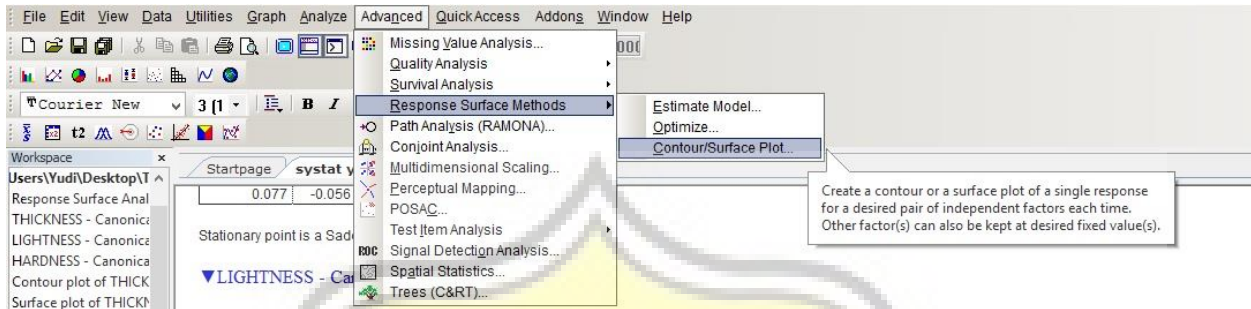
2) A dialog box will appear, and in the canonical tab. Add all of the parameters in the “Available response(s)” box to the “Selected response(s)” box by click **Add** button. Then, click **OK**.



7.4. Contour/ Surface Plot.

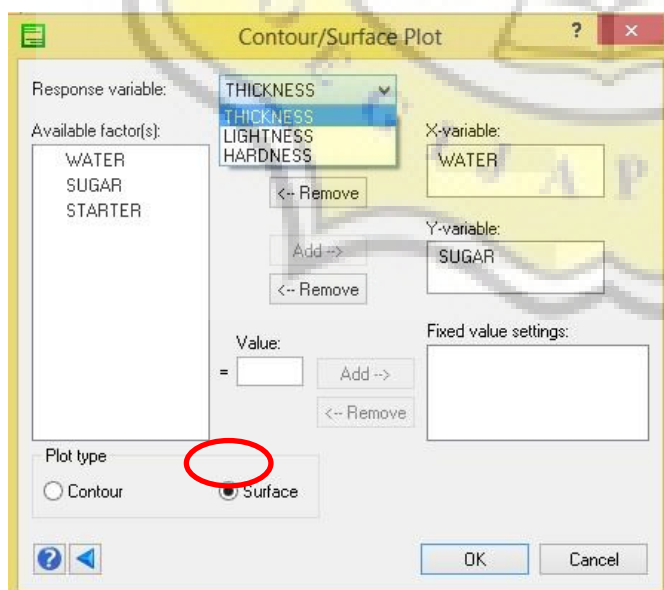
1) After finishing Optimization with Canonical Analysis in Response Surface Methods (RSM), the result analysis is made into graph to make it easier to determine the peak point of variable combinations (which signals the most optimal response). In order to do this,

block all the data, and then click “**Advanced > Response Surface Methods > Contour/Surface Plot**”



2) As the graph is only explain about the correlation between two variables towards a response. There will be 9 graphs generated in this experiment, with the combinations stated in the table below. Then, each of the combination is generated to the “**Contour/Surface Plot**” dialog box, with the “**Surface**” Plot Type. Then, click **OK**

Graph	X-variable	Y-variable	Response variable
1	Thickness	Water	Sugar
2	Thickness	Water	Starter
3	Thickness	Sugar	Starter
4	Lightness	Water	Sugar
5	Lightness	Water	Starter
6	Lightness	Sugar	Starter
7	Hardness	Water	Sugar
8	Hardness	Water	Starter
9	Hardness	Sugar	Starter



7.5. Result of Model Estimation of Thickness Response Using SYSTAT 12.0

Dependent Variable : THICKNESS

N : 400

Multiple R : 0.690

Squared Multiple R : 0.477

Adjusted Squared Multiple R : 0.465

Standard Error of Estimate : 0.252

Estimates of the Regression Coefficients				
Effect	Coefficient	Standard Error	t	p-value
CONSTANT	1.457	0.036	40.949	0.000
WATER	0.177	0.023	7.691	0.000
SUGAR	0.038	0.023	1.651	0.100
STARTER	0.010	0.025	0.388	0.699
WATER*WATER	-0.551	0.048	-11.544	0.000
SUGAR*SUGAR	-0.394	0.048	-8.250	0.000
STARTER*STARTER	0.075	0.048	1.541	0.124
WATER*SUGAR	0.400	0.050	7.945	0.000
SUGAR*STARTER	-0.026	0.056	-0.465	0.642
WATER*STARTER	-0.050	0.056	-0.887	0.376

Confidence Interval of the Regression Coefficients			
Effect	Coefficient	95.00% Confidence Interval	
		Upper	Lower
CONSTANT	1.457	1.387	1.527
WATER	0.177	0.132	0.223
SUGAR	0.038	-0.007	0.083
STARTER	0.010	-0.039	0.058
WATER*WATER	-0.551	-0.645	-0.457
SUGAR*SUGAR	-0.394	-0.487	-0.300
STARTER*STARTER	0.075	-0.021	0.170
WATER*SUGAR	0.400	0.301	0.499
SUGAR*STARTER	-0.026	-0.136	0.084
WATER*STARTER	-0.050	-0.159	0.060

Analysis of Variance					
Source	df	Type I SS	Mean Squares	F-ratio	p-value
Regression	9	22.643	2.516	39.465	0.000
Linear	3	3.900	1.300	20.390	0.000
Quadratic	3	14.655	4.885	76.630	0.000
Interaction	3	4.088	1.363	21.376	0.000
Residual Error	390	24.863	0.064		
Total Error	399	47.506			

Lack of Fit Test					
Source	df	SS	Mean Squares	F-ratio	p-value
Lack of Fit	5	11.402	2.280	65.221	0.000
Pure Error	385	13.461	0.035		
Residual Error	390	24.863	0.064		

Regression Coefficients for Uncoded Factors	
Effect	Coefficient
CONSTANT	-1.511
WATER	2.907
SUGAR	0.001
STARTER	-0.002
WATER*WATER	-0.781
SUGAR*SUGAR	0.000
STARTER*STARTER	0.000
WATER*SUGAR	0.004
SUGAR*STARTER	0.000
WATER*STARTER	-0.001

7.6. Result of Model Estimation of Lightness Response Using SYSTAT 12.0

Dependent Variable : LIGHTNESS
N : 400

Multiple R : 0.372
Squared Multiple R : 0.138
Adjusted Squared Multiple R : 0.118
Standard Error of Estimate : 4.593

Estimates of the Regression Coefficients				
Effect	Coefficient	Standard Error	t	p-value
CONSTANT	51.169	0.647	79.077	0.000
WATER	1.318	0.419	3.143	0.002
SUGAR	-0.394	0.419	-0.940	0.348
STARTER	-0.074	0.447	-0.166	0.868
WATER*WATER	5.534	0.868	6.375	0.000
SUGAR*SUGAR	4.686	0.868	5.398	0.000
STARTER*STARTER	2.632	0.881	2.989	0.003
WATER*SUGAR	-0.998	0.917	-1.089	0.277
SUGAR*STARTER	-0.651	1.016	-0.641	0.522
WATER*STARTER	-0.728	1.016	-0.716	0.474

Confidence Interval of the Regression Coefficients			
Effect	Coefficient	95.00% Confidence Interval	
		Upper	Lower
CONSTANT	51.169	49.897	52.441
WATER	1.318	0.494	2.142
SUGAR	-0.394	-1.218	0.430
STARTER	-0.074	-0.953	0.805
WATER*WATER	5.534	3.827	7.240
SUGAR*SUGAR	4.686	2.979	6.392
STARTER*STARTER	2.632	0.901	4.363
WATER*SUGAR	-0.998	-2.800	0.804
SUGAR*STARTER	-0.651	-2.649	1.347
WATER*STARTER	-0.728	-2.726	1.270

Analysis of Variance					
Source	df	Type I SS	Mean Squares	F-ratio	p-value
Regression	9	1,318.107	146.456	6.943	0.000
Linear	3	225.545	75.182	3.564	0.014
Quadratic	3	1,048.053	349.351	16.560	0.000
Interaction	3	44.510	14.837	0.703	0.551
Residual Error	390	8,227.243	21.095		
Total Error	399	9,545.351			

Lack of Fit Test					
Source	df	SS	Mean Squares	F-ratio	p-value
Lack of Fit	5	427.095	85.419	4.216	0.001
Pure Error	385	7,800.148	20.260		
Residual Error	390	8,227.243	21.095		

Regression Coefficients for Uncoded Factors	
Effect	Coefficient
CONSTANT	92.793
WATER	-26.324
SUGAR	-0.061
STARTER	-0.108
WATER*WATER	7.842
SUGAR*SUGAR	0.000
STARTER*STARTER	0.000
WATER*SUGAR	-0.009
SUGAR*STARTER	0.000
WATER*STARTER	-0.009

7.7. Result of Model Estimation of Hardness Response Using SYSTAT 12.0

Dependent Variable : HARDNESS

N : 400

Multiple R : 0.493

Squared Multiple R : 0.243

Adjusted Squared Multiple R : 0.225

Standard Error of Estimate : 587.866

Estimates of the Regression Coefficients			
Effect	Coefficient	Standard Error	p-value
CONSTANT	753.363	82.821	9.096 0.000
WATER	106.414	53.667	1.983 0.048
SUGAR	-271.283	53.667	-5.055 0.000
STARTER	66.364	57.202	1.160 0.247
WATER*WATER	574.780	111.102	5.173 0.000
SUGAR*SUGAR	720.148	111.102	6.482 0.000
STARTER*STARTER	97.607	112.713	0.866 0.387
WATER*SUGAR	-575.451	117.323	-4.905 0.000
SUGAR*STARTER	-341.445	130.057	-2.625 0.009
WATER*STARTER	-112.651	130.057	-0.866 0.387

Confidence Interval of the Regression Coefficients			
Effect	Coefficient	95.00% Confidence Interval	
		Upper	Lower
CONSTANT	753.363	590.531	916.194
WATER	106.414	0.901	211.927
SUGAR	-271.283	-376.796	-165.769
STARTER	66.364	-46.099	178.826
WATER*WATER	574.780	356.346	793.213
SUGAR*SUGAR	720.148	501.714	938.582
STARTER*STARTER	97.607	-123.993	319.208
WATER*SUGAR	-575.451	-806.115	-344.787
SUGAR*STARTER	-341.445	-597.145	-85.745
WATER*STARTER	-112.651	-368.351	143.049

Analysis of Variance					
Source	df	Type I SS	Mean Squares	F-ratio	p-value
Regression	9	43,220,739.752	4,802,304.417	13.896	0.000
Linear	3	11,659,762.202	3,886,587.401	11.246	0.000
Quadratic	3	20,605,773.395	6,868,591.132	19.875	0.000
Interaction	3	10,955,204.154	3,651,734.718	10.567	0.000
Residual Error	390	1.348E+008	345,586.693		
Total Error	399	1.780E+008			

Lack of Fit Test					
Source	df	SS	Mean Squares	F-ratio	p-value
Lack of Fit	5	36,378,191.277	7,275,638.255	28.466	0.000
Pure Error	385	98,400,619.117	255,586.024		
Residual Error	390	1.348E+008	345,586.693		

Regression Coefficients for Uncoded Factors	
Effect	Coefficient
CONSTANT	2,260.087
WATER	-1,997.011
SUGAR	1.562
STARTER	2.962

Regression Coefficients for Uncoded Factors	
Effect	Coefficient
WATER*WATER	814.597
SUGAR*SUGAR	0.045
STARTER*STARTER	0.011
WATER*SUGAR	-5.437
SUGAR*STARTER	-0.029
WATER*STARTER	-1.437

7.8 Canonical Analysis of Thickness

Factor	Stationary Point	
	Coded	Uncoded
WATER	0.216	2.182
SUGAR	0.157	169.810
STARTER	0.035	225.460

Optimal response = 1.479 with 95% confidence interval (1.413,1.545)

Eigenvalues and Eigenvectors			
Eigenvalues	Eigenvectors		
	WATER	SUGAR	STARTER
-0.688	0.827	-0.562	0.017
-0.259	-0.560	-0.825	-0.074
0.077	-0.056	-0.051	0.997

Stationary point is a Saddle Point.

7.8 Canonical Analysis of Thickness

Factor	Stationary Point	
	Coded	Uncoded
WATER	-0.116	1.902
SUGAR	0.030	153.751
STARTER	0.002	222.306

Optimal response = 51.086 with 95% confidence interval (49.828,52.344)

Eigenvalues and Eigenvectors			
Eigenvalues	Eigenvectors		
	WATER	SUGAR	STARTER
5.777	0.915	-0.399	-0.065
4.557	-0.377	-0.899	0.223
2.517	0.147	0.180	0.973

Stationary point is Minimum.

7.9 Canonical Analysis of Hardness

Factor	Stationary Point	
	Coded	Uncoded
WATER	-0.007	1.994
SUGAR	0.178	172.430
STARTER	-0.032	219.124

Optimal response = 727.788 with 95% confidence interval (569.396,886.179)

Eigenvalues and Eigenvectors			
Eigenvalues	Eigenvectors		
	WATER	SUGAR	STARTER
956.414	0.586	-0.801	0.121
416.671	-0.767	0.500	0.403
19.450	0.262	0.329	0.907

Stationary point is Minimum.

7.10. Design and Optimization in Organic Synthesis Book Screen Capture

259

Table 12.3: Summary of Central Composite Designs*

Number of variables:	2	3	4	5	5	6	6
Factor points:							
Design	2^2	2^3	2^4	2^{5-1}	2^5	2^{6-1}	2^6
Number of factor points, N_F	4	8	16	16	32	32	64
Center points:							
Number of center points, N_0							
Uniform precision	5	6	7	6	10	9	15
Orthogonality	8	9	12	10	17	15	24
Axial points:							
Value of α	1.414	1.682	2.000	2.000	2.378	2.378	2.828
Number of axial points, N_A	4	6	8	10	10	12	12
Total number of experiments, N:							
Uniform precision	13	20	31	32	52	53	91
Orthogonality	16	23	36	36	59	59	100

* Data are taken from Box and Hunter[4]