Response Surface Designs

Q.1. A response surface was fit relating 3 factors (oil/ethanol ratio, catalyst amount (KOH), and reaction time) to mass yield of biodiesel fuel, using a central composite design. The data and regression results are given below (the analysis was based on coded values with axial points at $\alpha = \pm 1.68$). The model fit is:

$$E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2$$

Oil:EtOH	KOH	Time	Yield	x1	x2	x3	x1x2	x1x3	x2x3	x1^2	x2^2	x3^2
10.2	1.5	60	81.67	-1	-1	-1	1	1	1	1	1	1
10.2	1.5	120	80.06	-1	-1	1	1	-1	-1	1	1	1
10.2	2	60	67.01	-1	1	-1	-1	1	-1	1	1	1
10.2	2	120	75.3	-1	1	1	-1	-1	1	1	1	1
11.8	1.5	60	85.75	1	-1	-1	-1	-1	1	1	1	1
11.8	1.5	120	84.03	1	-1	1	-1	1	-1	1	1	1
11.8	2	60	68.95	1	1	-1	1	-1	-1	1	1	1
11.8	2	120	78.97	1	1	1	1	1	1	1	1	1
9.656	1.75	90	74.68	-1.68	0	0	0	0	0	2.8224	0	0
12.344	1.75	90	83.39	1.68	0	0	0	0	0	2.8224	0	0
11	1.33	90	80.49	0	-1.68	0	0	0	0	0	2.8224	0
11	2.17	90	72.48	0	1.68	0	0	0	0	0	2.8224	0
11	1.75	39.6	74.64	0	0	-1.68	0	0	0	0	0	2.8224
11	1.75	140.4	75.18	0	0	1.68	0	0	0	0	0	2.8224
11	1.75	90	86.32	0	0	0	0	0	0	0	0	0
11	1.75	90	86.32	0	0	0	0	0	0	0	0	0
11	1.75	90	85.29	0	0	0	0	0	0	0	0	0
11	1.75	90	85.06	0	0	0	0	0	0	0	0	0

ANOVA

	df	SS	MS	F	gnificance
Regressio	9	590.14	65.57	11.30	0.0012
Residual	8	46.43	5.80		
Total	17	636.57			

	Coefficients	andard Err	t Stat	P-value
Intercept	85.67	1.20	71.24	0.0000
x1	2.07	0.65	3.18	0.0130
x2	-4.01	0.65	-6.15	0.0003
x3	1.16	0.65	1.79	0.1120
x1x2	-0.31	0.85	-0.36	0.7295
x1x3	0.20	0.85	0.24	0.8181
x2x3	2.71	0.85	3.18	0.0131
x1^2	-2.06	0.68	-3.03	0.0162
x2^2	-2.96	0.68	-4.37	0.0024
x3^2	-3.52	0.68	-5.19	0.0008

p.1.a. Give the fitted value when (the original units of) oil/ethanol ratio is 11, KOH catalyst is 1.75, and reaction time is 90.

p.1.b. Make use of the 4 center points to compute SS(Pure Error) and SS(Lack-of-Fit), and test for lack of fit, where:

$$SSPE = \sum_{i=1}^{c} \sum_{j=1}^{n_i} \left(Y_{ij} - \overline{Y}_{i\bullet} \right)^2 \qquad SSLF = SSE - SSPE \qquad c \equiv \text{\# of distinct levels of predictors} \quad \text{df(PE)} = n - c$$

Test Statistic: _____ Conclude the model does not fit if the test statistic is in the range _____

p.1.c. What values of the 3 factors (in their original units) will maximize the yield? Note:

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} \quad \text{where: } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} b_{11} & b_{12}/2 & b_{13}/2 \\ b_{12}/2 & b_{22} & b_{23}/2 \\ b_{13}/2 & b_{23}/2 & b_{33} \end{bmatrix}$$

b		B				INV(B)		
2.07		-2.06	-0.15	0.10		-0.488	0.023	-0.005
-4.01		-0.15	-2.96	1.35		0.023	-0.410	-0.157
1.16		0.10	1.35	-3.52		-0.005	-0.157	-0.345