SOLUTION ABSTRACT

TEAM ID: OP-007

ABSTRACT SUBMISSION CODE: aeeocqey

Concise problem statement: Identifying the maximum rate of formation of B and the corresponding operating temperature (in the range of 200-250 K) and concentration (in the range of 15-25 mol/cc) with minimum no. of simulations using response surface methodology.

Solution approach: Since a key objective was to minimise the number of simulations, a design of experiments approach was adopted to choose apt values of temperature and concentration. Hence, a **modified 3-level full factorial method** was used. No. of factors was set at 2 (signifying temperature and concentration). Level '0'signifies the low values the factor could take, '1'- intermediate and '2'- high in 200-250K and 15-25 mol/cc. Reaction rate was set as the response variable. An extra reading was taken at 150K, 0 mol/cc to evaluate out-of-range behaviour.

Table 1: Data points at which experiments were simulated

Temperature(in K)	TRep *	Concentration (mol/cc)	CRep*	Rate
200	0	15	0	45.2561
200	0	19	1	59.7061
200	0	23	2	67.1814
230	1	17	0	79.3134
230	1	21	1	82.6457
230	1	25	2	79.9068
250	2	15	0	80.2117
250	2	20	1	82.2948
250	2	25	2	73.3592
150	Not applicable	0	Not applicable	-217.4055

*TRep- corresponding temperature level

*CRep- corresponding concentration level

The values were subjected to multivariate linear regression on MATLAB. Amongst all regression functions tested, stepwise quadratic was zeroed in as the best fit due to low RMSE value of 0.195. Regression table and ANOVA table of stepwise quadratic model are given below as Table 2 and Table 3 respectively.

Table 2: Regression table for stepwise quadratic regression model

	Estimate	SE	tStat	pValue
Intercept	-1085.3	10.082	-107.65	4.4657e-08
T	7.8818	0.10036	78.539	1.5752e-07
C	22.646	0.14215	159.31	9.3113e-09
T:C	-0.059753	0.00088602	-67.44	2.8963e-07
T^2	-0.013971	0.00022613	-61.786	4.1099e-07
C^2	-0.20983	0.0042285	-49.622	9.8693e-07

Number of observations: 10, Error degrees of freedom: 4
Root Mean Squared Error: 0.195
R-squared: 1, Adjusted R-Squared: 1
F-statistic vs. constant model: 4.05e+05, p-value = 1.71e-11

Table 3: ANOVA for the chosen stepwise quadratic regression model.

	SumSq	DF	MeanSq	F	pValue
T	975.25	1	975.25	25691	9.088e-09
C	59.612	1	59.612	1570.4	2.4227e-06
T:C	172.65	1	172.65	4548.2	2.8963e-07
T^2	144.91	1	144.91	3817.5	4.1099e-07
C^2	93.47	1	93.47	2462.3	9.8693e-07
Error	0.15184	4	0.03796		

Regression model: The model obtained was of the form **rate ~ 1 + temp*conc + temp^2 + conc^2**.
When converted from Wilkinson's notation and after plugging in estimated coefficients from the regression table, the final regression equation (fitted model) was obtained as follows:

Rate of formation of B= $-1085.3 - 0.059753*T*C - 0.013971*T^2 - 0.20983*C^2 + 7.8818*T + 22.646*C$ (Eq 1)
where T= temperature(in K) and C= concentration of A (mol/cc).

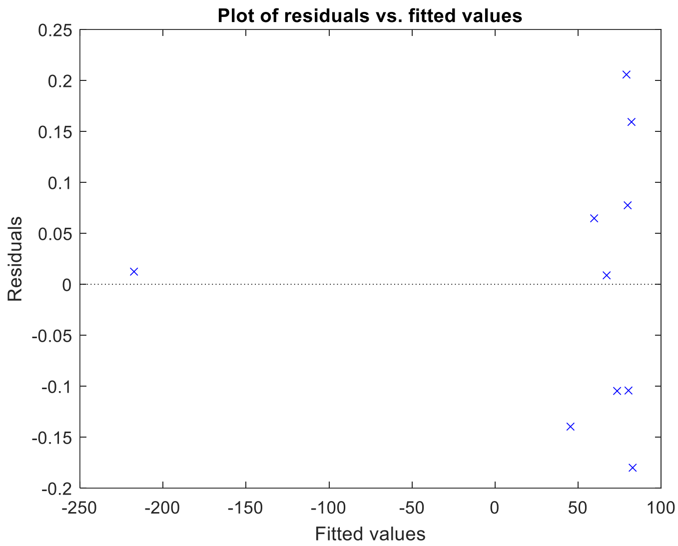

Fig 1: Plot of residuals vs fitted values

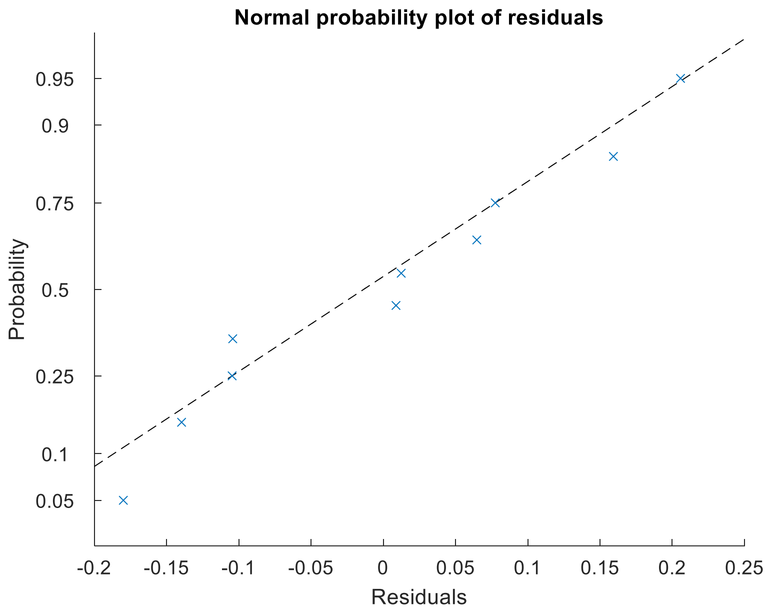

Fig 2: Normal Probability plot for residuals

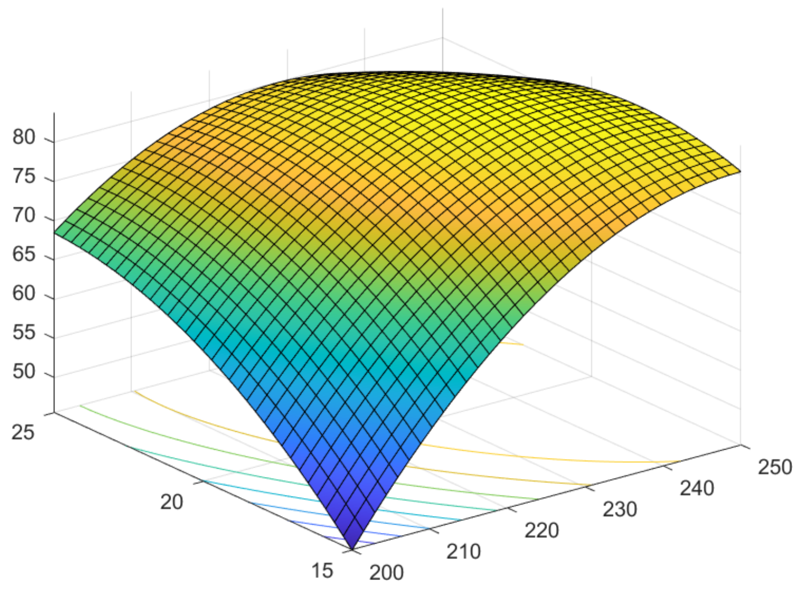

Fig 3: Surface plot rate over temperature and concentration

Obtaining partial derivatives of Eq 1 with respect to temperature and concentration and equating them to zero gives a point of extremity at- temperature= 239.6490 K and concentration= 19.8405 mol/cc. The corresponding value of rate of formation of B= 83.7864.

Let g= ∂(rate)/∂(T) = 7.8818 - 0.0279*temp - 0.0598*conc

i= ∂(g)/∂(T) = -0.0279

h= ∂(rate)/∂(C) = 22.6460 - 0.0598*temp - 0.4197*conc

j= ∂(h)/∂(C) = -0.4197

When g=h=0, a point of local extremum is obtained at temperature= 239.6490 K and concentration= 19.8405 mol/cc. The corresponding value of rate of formation of B= 83.7864. Since I and j are both negative in those points, a local maxima is observed and hence the maximum rate of formation of B is obtained with those temperature and concentration values.

Conclusion: The simulator was used to perform 10 experiments in total. A stepwise quadratic regression approach was adopted. Regression equation:
Rate of formation of B= **−1085.3 -0.059753*T*C- 0.013971*T^2 -0.20983*C^2 +7.8818*T +22.646*C**
where T= temperature(in K) and C= concentration of A (mol/cc)

Max rate of formation of B= 83.7864
Operating temperature= 239.6490 K
Concentration of A= 19.8405 mol/cc

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APPENDIX

MATLAB Code used:

```
modelspec= 'rate~temp+conc';

mdl= fitlm(optimizer);

mdls=stepwiselm(optimizer,'interactions');%to
study interaction between variables

mdl3=stepwiselm(optimizer,'quadratic','ResponseVar
','rate','Upper','quadratic')

f=@(temp,conc)-1085.3-0.059753*temp*conc-
0.013971*temp^(2) -
0.20983*conc^(2)+7.8818*temp+22.646*conc;

fsurf(f,[200 250 15 25],
'ShowContours','on');%generates surface plots
syms temp conc rate

rate= -1085.3-0.059753*temp*conc-0.013971*temp^2 -
0.20983*conc^2+7.8818*temp+22.646*conc;

g= diff(rate,temp);%differentiates rate wrt
temperature

h=diff(rate,conc); %differentiates rate wrt
concentration

eqns=[g==0,h==0];

i=diff(g,temp)

j=diff(h,conc)
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```
Sol= solve(eqns,[temp conc]);
temp=Sol.temp; ;%required operating temperature
conc=Sol.conc; %required operating concentration
subs(rate);% required rate of formation of B
subs(i);
subs(j);
plotResiduals(mdl3,'probability');
%plotResiduals(mdl3,'fitted')
%plotResiduals(mdl3)
anova(mdl3);%performs ANOVA for model
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