Modelling

Experimental approach modeling and statistic

For better interpretation of our experimental data we utilized the software Statistica version 7.0, using the Central Composite Design (CCD).

1. **Central Composite Design**

A Central Composite Design to k factors, codified as (x1, ..., xk), is formed in three parts:

One called factorial (or cubic) containing a total of n_{fat} coordinate points xi = -1 ou xi = +1, for all i = 1 ..., k;

A axial part (or in star), formed by n_{ax} = 2k points with all coordinates null, but one,which is equal to a determined α value (or -α);

A total of n_{centr} assays done in the central point, where x1 =....xk = 0 (Barros Neto, 1995).

To do the CCD, is needed to define how is going to be each part. One design with k = 3 is showed in the figure 3, where we can see the cubic, star and center point parts.

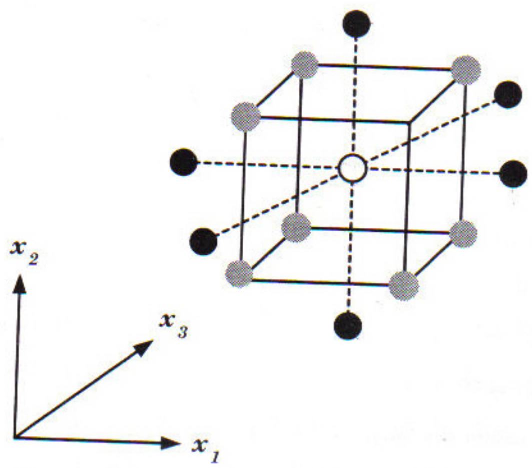

Figure 3 – CCD for three factors. (Barros Neto, 1995).

The cubic points are identical likely a two-level factorial. The axial points are dependant of α value which can vary from 1 to k½. To choose the best α value we utilize the rotability concept as criteria. Following this concept, a feasible design can be achieved if the estimative variance depends upon only on the distance to the central point. The mathematical criteria of rotability is that α = k¼. Therefore as seen in the table 1, the proposed CCD is a process (α = 3¼ = ±1,682), five assays in the central point can stabilize the variance in the previewed answer, giving a pure measuring error.

Tabela 1 – Factorial CCD used.

Part of Design	Assay	X_1	X_2	X_3
Factorial	1	-1	-1	-1
	2	1	-1	-1
	3	-1	1	-1
	4	1	1	-1
	5	-1	-1	1
	6	1	-1	1
	7	-1	1	1
	8	1	1	1
Axial	9	-1,682	0	0
	10	1,682	0	0
	11	0	-1,682	0
	12	0	1,682	0
	13	0	0	-1,682
	14	0	0	1,682
Central	15	0	0	0
	16	0	0	0
	17	0	0	0
	18	0	0	0
	19	0	0	0

In the table 2 we describe the utilized factors with their respective values to the table 1.

Table 2 –Factors utilized in the CCD factorial with their respective levels.

Factors	Chossed values	Levels from the statistic design

	Minimum	Maximum					
	-1,68	+1,68	-1,68	-1	0	+1	+1,68
Temperature(°C)	25	40	25	28	32,5	37	40
pH	4,3	7,6	4,3	5	6	7	7,6
Oil concentration (%)	1,5	18,5	1,5	5	10	15	18,5

To optimize work (Table 3), as written in the item 3.5, we have made an experimental modeling using the factors pH, temperature and oil concentration, having as feedback the oil degradation rate in different conditions, randomly.

The residual quadratic sum left by the model can be decomposed in two parts: one caused by random events, and other due to the lack of adjustments in the model. The term will give a random measurement of the error and can is called quadratic sum due to the pure error (SQ_{ep}). The second part depends upon our model and follows the quadratic sum due to the lack of adjustment (SQ_{faj}) (Barros Neto, 1995).

Dividing these quadratic sums by their degrees of freedom, we end up with the average in which values can be compared to evaluate the lack of model adjustment. We can use the test F in the ratio MQ_{faj}/ MQ_{ep} to evaluate IF the model is well suited to our observations. High values of MQ_{faj}/ MQ_{ep} indicate lack of adjustment showing that the model is not adequate (Barros Neto, 1995).

Tabela 3: Experimental variance analisys

Variation source	**Quadratic sum**	**Degree of freedom**	**Quadratic average**
Regressão	3805.69	1	3805.69
Resíduos	1166,04	17	68,58
Falta de ajuste	345,94	7	49,42
Erro puro	820,10	9	91,12
Total	4971,73	18	
% of explanation			76,54%
% explained variation			83,50%

The porcentage of explanation indicates how much of variation phenomena is explained while the explained variation percentage is how can it be explained by the proposed model (Barros Neto, 1995).

To validate the experimental we used the T (equation 1), where is observed that if the quadratic average of regression is very superior than the quadratic average of the residues then the the regression is significative and the model is valid.

Equation 1: T test: regression and residues

As demonstrated in the table 5, there are variables pointing to the lack of experimental adjustments and pure error. On top of that we made the T test. As described in the equation 7, the quadratic average is lower than the experimental error quadratic average due to the lack of adjust, being the values relatively close, which shows is not possible to improve the model.

Equation 2: T test analysis - lack of adjustment and pure error

As the regression result, we obtained a quadratic equation that models the influence of pH (pH), temperature (temp) and oil concentration (oil) in the middle of the oil degradation rate (%Consumo):

$$\%Consumo = 697{,}124 + 31{,}29temp + 66{,}427pH + 6{,}111oil - 0{,}435temp^2 - 3{,}059pH^2$$
$$+ 0{,}305oil^2 - 0{,}259temp.pH - 0{,}151temp.oil - 1{,}456pH.oil$$

This equation can be better interpreted when analyzed through level-surface graphics. In the figure 8 we have the analysis of pH and temperature as the rate of consumption. In this graphic representation the more red is the region better are the results. As shown the high pH more narrow is the temperature we can work, while the oil degradation goes up significatively.

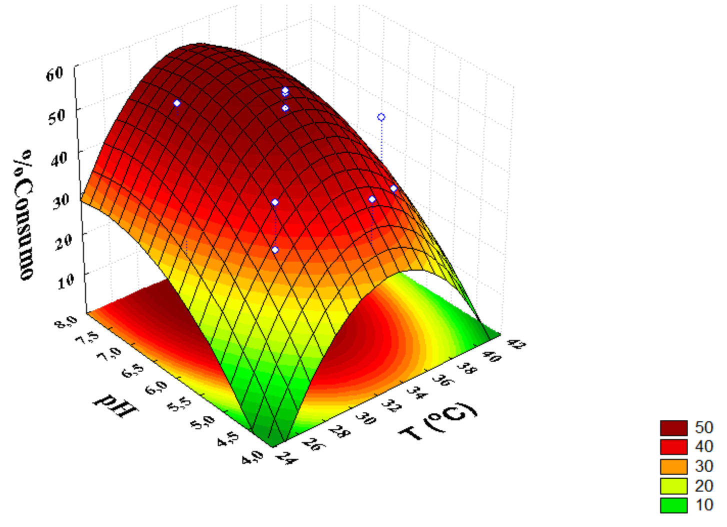

Figure 4: pH X temperature in the oil degradation.

In the figure 5, we have as analysis point the relation between oil concentration and consumption rate. The temperature range is very large and the increase percentage of degradation is observed if only high concentrations of oil is present in the media.

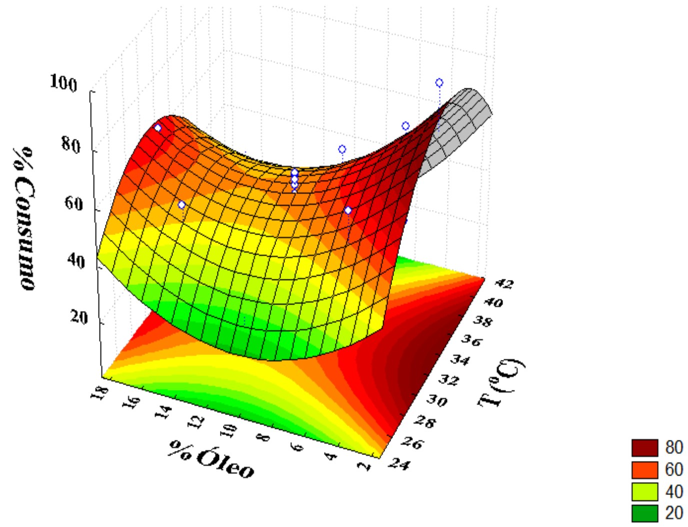

Figure 5: oil concentration X temperature affecting the degradation.

In the figure 6, we have points taking in account the oil concentration and pH affecting the oil consumption. The pH range is very broad and the increasing of degradation is noted only if there is high oil concentration in the media.

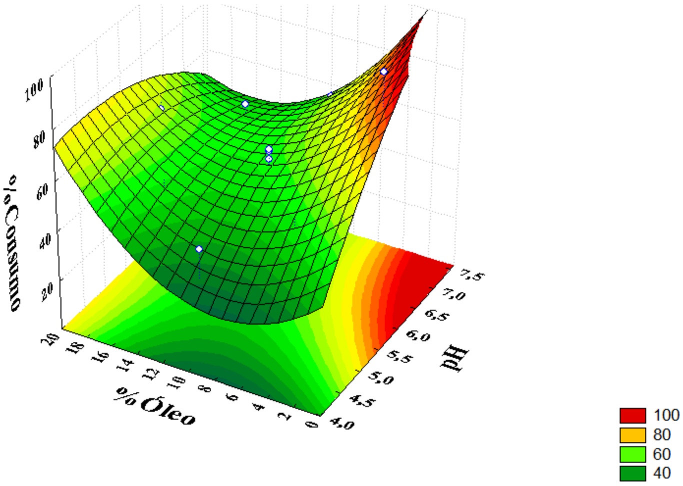

Figure 6: oil concentration X pH affecting used frying oil degradation.

After applying the equation we have the following best conditions to work: temperature 32,5°C, pH=6,00 and10% oil concentration.