A Cost-Effective and Common Sensical Approach to Batch Process Optimization - an Industrial Case-Study

Prasanth Chandrahasan
Sheetal K. Bafna

Texas A&M University

INTRODUCTION

This paper introduces the concept of heuristic model based optimization. Heuristic model can be applied to processes which cannot be derived from first principles or which lacks enough experimental data. A heuristic model is defined as any function derived from the process parameters which represent a process approximately but appropriately. This concept is illustrated through two case studies, both taken from the manufacture of Cyper Methric Acid Chloride (CMAC), an agrochemical.

The first case study is about the yield dependency of a crucial stage in CMAC manufacture (2CB stage) on the reaction time of an upstream stage (TBA stage). It was found that more the reaction temperature of TBA less is the yield of the 2CB stage, the actual reasons for which is unknown. This relation but cannot be modeled from first principles. Hence we make use of a heuristic model to arrive at an approximate process model called TWAT model, optimizing which was equivalent to optimizing the actual process. It was found from the results of the optimization that there can be potential financial savings if the results were implemented. And the capital investment required is nil.

The second case study involves no chemical reaction. The 2CB reaction produces a tarry waste which sticks to the impeller shaft of the reaction vessel in which the reaction is carried out. Cleaning the reactor after every batch increases the reaction yield, but increases the batch time. Also this relationship of waste accumulation and reduction in reaction yield cannot be derived from first principles. Here also a heuristic model was derived for the frequency of reactor cleaning and optimized.

HEURISTIC MODEL

CONCEPT OF HEURISTIC MODEL

The term “Heuristic Model” here is confined only to a chemical process and has the general form,

$$M = f(x_1, x_2 \ldots x_N)$$

where M is a dependent chemical parameter to be optimized which is a function of any other parameter(s) $x_1, x_2 \ldots x_N$. Heuristic model is so called because,

1. It need not have a physical significance
2. The structure of the function is entirely dependent on the process under consideration

Heuristic model is any relationship between the given process parameters which is,

1. Approximate
2. Appropriate

The model is appropriate in that it represents the trend shown by process variables. It is also approximate in that it is not a derived considering all the dependencies between the variables under consideration. From a single chemical process any number of functions can be derived. The only qualification for the selection of the specific heuristic model is that it has to represent the behavior of the parameters and that it has to behave as a function.

For example, in the first case study, the relationship between the reaction time and temperature of a process (TBA) and the reaction yield of a downstream process (2CB)is given by table,

Table 1: TBA time temperature relation with 2CB yield

TBA MAINTANING TEMPERATURE			2CB YIELD (KGS)
67°C	85°C	97°C	

1.5	3	3.5	1050
12	0	2	1150
18	0	1	1200
1.5	0	4.5	1020

Thus from the table 1, if the temperature maintaining were done at a temperature of 67°C for 1.5 hours and for 3 hours at 85°C and 97°C for 3.5 hours, the 2CB yield for a standard 5.2 kilo mole batch would be 1050 Kgs. This is the normally obtained yield. Where as if we maintain for 12 hours at 67°C and raise the temperature to 97°C and maintain for 2 hours, we get a yield of 1150 kilograms at 2CB stage for a standard 5.2 kilomole batch size. The process parameters here are,

1. 2CB yield
2. TBA reaction time
3. TBA reaction temperature

With these three parameters, any relationship can be created like,

1. Modulus of mean temperature minus original temperature
2. Temperature / time
3. Time squared / temperature
4. Temperature × weight average time (TWAT)

Let us see whether the second item qualifies to be a heuristic model. The relationship is given by

Table 2: 2CB yield versus Temperature time

Yield	Temperature/time
1020	66.222
1050	100.714
1150	54.0833
1200	100.722

It is evident that the there is no one-to-one relationship between the values and hence does not show any trend at all. So this relationship cannot be taken as a heuristic model. Now let us examine the last relationship – Temperature × weight average time (TWAT). The term Temperature weight average time means that time is weighted and multiplied with corresponding temperature. For example time weight % of 1.5 hours is given by 1.5 (1.5+3+3.5) where the denominator gives the total time maintained. Hence the Temperature × Weight average time for 1050 Kgs is given by the equation:

$$\text{TWAT for 1050} = \frac{(67*1.5+85*3+97*3.5)}{(1.5+3+3.5)}$$

This value as compared to the 2CB yields was found to be inversely related, as is evident from the table 3.

Table 3: TBA reaction temperature, 2CB yields and TWAT values

YIELD	67°C	85°C	97°C	TIME WEIGHT %			TWAT
1050	1.5	3	3.5	0.188	0.375	0.438	86.88
1150	12	0	2	0.857	0	0.143	71.29
1200	18	0	1	0.947	0	0.053	68.58
1020	1.5	0	4.5	0.250	0	0.750	89.50

The TWAT model hence qualifies as a heuristic model for the process under consideration.

The reason for selection of a heuristic model is either or both of the following,

1. The dependency of the various parameters cannot be derived from first principles
2. There is too little data available to satisfactorily find the relation between parameters

The actual reason for temperature dependency of 2CB reaction is unknown. But the TWAT model gives an approximate method for connecting temperature, time and yield. The generalized procedure for optimization involving heuristic model envisaged here is,

1. Identification of processes where the heuristic model method can be applied
2. Collection of relevant plant data
3. Selection of appropriate heuristic model
4. Fitting heuristic model to an equation
5. Selection of constraints, if any
6. Input to any standard optimizer
7. Output - this will be the optimized value

Though no general method for finding out the heuristic model can be described, the following will serve as an approximate guide,

1. List all the parameters involved
2. If one or more parameters are functions of any other parameters, list the latter in place of former
3. Now there will be two sets of values,
(a) Dependent parameter
(b) Independent parameter(s)
4. Try out different combinations which shows a trend
5. Select the one which shows a trend as the heuristic model

This project is all about the application of the heuristic model for optimizing chemical processes illustrated through two case studies. While both examples are part of the manufacture of the same chemical compound, they are unrelated in that the independent parameters optimized are different.

PROBLEM DEFINITION: TBA TIME OPTIMIZATION

Batch process optimization has been a long time issue of study and is classified into two types [Bonwin, 1998],

1. Achieved by changes in process parameters - done by a chemical engineer,
2. Achieved by change in process itself - done by a chemist.

Usually due to unsteady nature of market conditions, it is not possible to dedicate much time and money on the latter type of optimization. Hence the onus of improving the process falls on the chemical engineer, who also has to justify the resources used for improving the process. This case study showcases such a situation where the manufacturer was reluctant to spend more on a product which was about 15 years in production and fetched lower and lower profit margins year after year. This demanded process improvements to reduce the product price. Lab scale improvement work has long been ceased and the only way to improve on the process was in the plant directly. The product fetched great demand and thus any change which affects the production rate was also not possible. This provides an ideal situation for the concepts outlined in this paper – a heuristic model based method to optimize the process.

The data required for doing the optimization was obtained when the plant was in shutdown stage. Being a batch process, only certain sections of the plant were under shutdown and thus the production was slowed down. This enabled extraction of plant data by varying parameters. It is to be noted that unlike a laboratory experiment, the data points are few in number.

BASIC CHEMISTRY AND CHEMICAL REACTION

The production process under consideration is that of cypermethric acid chloride (CMAC) also known as D.V acid chloride (empirical formula : C8H9Cl3O, chemical name : 3-(2, 2-dichlorovinyl)-2, 2-dimethyl cyclopropane-1-carboxylic acid chloride).

It is a pesticide intermediate which is used for the manufacture of the following pesticides:

1. Cypermethrin
2. Permethrin
3. Alpha cypermethrin
4. Beta cypermethrin
5. Gamma cypermethrin

The production of CMAC is done in six consecutive stages as follows. A stage usually refers to a unit process and unit operations like distillation are not normally denoted by the term.

1. Tetra chloro butyro nitrile (TBN)
2. Tetra chloro butyric acid (TBA)
3. 2 Tetra chloro cyclo butanone (2CB)
4. Permethric acid (PA)
5. Cypermethric acid (CMA)
6. Cypermethric acid chloride (CMAC)

The starting raw materials (for TBN stage) are acrylonitrile and carbon tetra chloride. There are two processes under consideration here,

1. Tetra chloro butyric acid (TBA)
2. 2 Tetra chloro cyclobutanone (2CB)

About TBA reaction

The conversion of TBN (tetra chloride butyro nitrile)to TBA (tetra chloro butyric acid)is a hydrolysis reaction done using H+ ions in a mineral acid. The first stage of hydrolysis is the conversion of TBN to TBAmide, which is then converted to TBA.

$$\text{TBN} + \text{HCl} \longrightarrow \text{TBAmide} + H_2O \longrightarrow \text{TBA}$$

(This is just a schematic representation of the reaction and is not balanced)

REACTION CONDITIONS

The reaction is done is a glass lined vessel. Around 32.4 kilo moles of H+ ions is taken (as HCl and makeup H_2SO_4)and TBN fed over a period of about 5 hours at a temperature of 67 ±1°C. The batch size is 18 kilo moles of TBN and total H+ ions correspond to 1.8 kilo moles per mole of TBN. The reaction is exothermic at all temperatures and does not need heating once initiated. Once initiated, to keep the reaction under control, small amounts of water are send through the reactor jacket, known as "cooling shocks". The frequency and intensity of "cooling shocks" depends on the time for which the control valve in the cooling water line keeps itself open which is in turn dependent on the temperature of reaction mass. After the feeding is over, the reaction mass contains TBN, TBA, and TBAmide, the proportion of which is unknown since it is not measured. After the feeding, reaction mass is maintained for a minimum of 1.5 hours at the same temperature (67± 1°C) and is sampled for TBN and TBAmide content. The usual average content is around 0.2% by weight of TBN and 35% by weight of TBAmide. The temperature is then raised to a value higher than 67°C so as to reduce the TBAmide content to around 0.2% by volume, which is the maximum possible conversion since the rest will be impurities. The standard time cycle for TBA stage can is as follows

1. HCl receiving in reactor: 0.5 Hours
2. H_2SO_4 makeup for normality: 0.25 Hours
3. Heating to feeding temperature: 0.75 Hours
4. Feeding: 5 Hours
5. Temperature raising & maintaining: 10 Hours
6. Work up and transfer: 4 Hours
7. Total: 21.5 Hours

ABOUT 2CB REACTION

The 2CB process has been the trickiest stage in the entire process since it adds the maximum value to the product but has the least reaction yield (on a mole per mole basis). Hence it was always an area of interest since a small increase in the production rate would bring substantial savings to the cost. Needless to say, the stage was running at the maximum possible production rate and there was hardly any scope for improvement but with capital investment. The 2CB yield value has been more expressed in kilograms produced per standard batch size throughout the paper due to the simplicity of expression. In this process, the TBAC (Tetra chloro butyric acid chloride) and TEA (triethyl amine) are fed over a time period to a mixture of hexane and isobutylene where the latter is the reactant and the former is the medium. Various factors have been found out as the influencing factors for 2CB yield, provided that the feeding parameters remain the same out of which temperature of TBA reaction remains the most prominent one.

SIGNIFICANCE OF TEMPERATURE

The TBN to TBAmide reaction is an addition reaction while the TBAmide to TBA reaction is a hydrolysis reaction. The feeding temperature of 67 ± 1°C was foundout by laboratory trials during product development. The realtively long time cycle of TBA stage (21.5 hours) led to high temperature reaction trials at 105 ± 1°C. There was significant reduction in TBA time cycle but the 2CB yields obtained were lower. This led to the conclusion that there is a relation between TBA reaction temperature as well as 2CB yields, though the exact reason is still not known. It been hypothesized that at higher temperature either the TBA undergoes dissociation or that there is leaching of impurities. As practiced in the plant,we maintain for 1.5 hours at the feeding temperature and then at 85°C for 3 hours without sampling and then raised to 97°C for 3.5 hours minimum and sampled . If the amide content is 0.2% or less, batch is terminated or maintained further till it is achieved. These temperature values of 67°C, 85°C, 97°C and time values of 1.5 hours, 3 hours and 3.5 hours are purely judgmental. No mathematical explanation can be given for the selection of these values.

It is not easy to analytically derive an expression for TBA maintaining time and temperature to that of 2CB yield. Hence we resort to the optimization process involving heuristic model which approximates the relation between the three parameters as explained in the previous section.

PROCESS MODEL

The optimization strategy is as follows,

1. Find out the heuristic model which connects 2CB yield and TBA maintaining temperature and time
2. To set the constraints to optimization which will be time cycle and percentage of completion
3. Maximize the yield as the objective function through which the constraints will also be satisfied

STEP 1: TEMPERATURE - 2CB YIELD CORRELATION

To find a TBA maintaining (reaction) temperature and time and 2CB yield correlation. Old plant data was taken and analyzed. As described in chapter three, a heuristic model (called TWAT) was made and the data correlated as shown in table.

Table 4: TBA reaction temperature, 2CB yields and TWAT values

YIELD	67°C	85°C	97°C	TIME WEIGHT %			TWAT
1050	1.5	3	3.5	0.188	0.375	0.438	86.88
1150	12	0	2	0.857	0	0.143	71.29
1200	18	0	1	0.947	0	0.053	68.58
1020	1.5	0	4.5	0.250	0	0.750	89.50

STEP 2: TO FIND THE EQUATION CONNECTING TWAT AND 2CB YIELD

Linear, quadratic and cubic curves were fit which returned the values as shown in table.

Table 5: Linear,quadratic and cubic data fit to TWAT-Yield data

TWAT	Yield	Linear Model	Quadratic Model	Cubic Model
89.5	1020	1023.33959	1028.267343	1019.96
86.88	1050	1043.83737	1038.961049	1049.96
71.29	1150	1165.806982	1160.725639	1149.97
68.58	1200	1187.008884	1192.04706	1199.97
Standard Deviation	***	12.486	11.083	0.006924

The cubic model which accurately fit the data was taken as the basis for optimization, which is given as,

Yield = -0.044658(TWAT)^3 + 10.7839(TWAT) ^{3} - 871.459(TWAT) + 24649.9

This is the heuristic model connecting the TBA maintaining temperature, maintaining time and 2CB yield. The strategy is to optimize the heuristic model, which will tantamount to optimizing the actual process.

STEP 3: TO FIND THE KINETIC RATE CONSTANT OF REACTION

The final conversion of TBA has to be 99.9% or more (though actual conversion is 99.8%, assuming it to be 99.9% gives a more conservative value), hence it was necessary to calculate the conversions at different temperatures. Also the conversions after specific periods of time were also needed to be calculated. It was assumed that the reaction is first order, which is true for elementary reactions. For a irreversible unimolecular-type first-order reaction general procedure for integral method of analysis is given as.

$$A \longrightarrow \text{products}$$

$$-r_A = -dC_A$$
$$dT = kC_A$$

Integrating we get,

$$-\int_{C_{Ao}}^{C_A} \frac{dC_A}{C_A} = k\int_0^t dt$$

or

$$-\ln\frac{C_A}{C_{Ao}} = kt$$

Converting to volumes,

$$-\ln\frac{V_A}{V_{Ao}} = kt$$

Dropping the subscript “A”,

$$\frac{V}{V_o} = e^{kt}$$

But

$$\frac{V}{V_o} \quad = \quad \text{Extent of reaction completion}$$

=) Extent of reaction completion = e^{kt}

In this case since the reaction happens at three different temperatures,

Final reaction completion = $e^{k(t_1+t_2+t_3)}$

This equation is used for further calculations

To calculate the temperature dependency of rate constant, all the previous data was culled out and analyzed. The data analyzed was for two temperatures, for 67°C and for 80°C and is tabulated in table below

Rate constant calculation

Table 6: Temperature = 67°C

HRS	AMIDE CONTENT %	VOL	V_0/V	T-T0	$\text{Ln}(V_0/V)$	RATE CONSTANT(k)
0	47	1167.48	1	0	0	***
2	37	919.08	1.27027	2	0.23923	0.119614845
6	23	571.32	2.043478	6	0.714653	0.119108898

AVG k : 0.119362 HOUR^{-1}

Temperature = 80°C

HRS	AMIDE CONTENT %	VOL	V_0/V	T-T0	$\ln(V_0/V)$	RATE CONSTANT(k)
Batch I						
1.5	35.9	891.756	1	0	****	****
5	6.1	151.524	5.885246	5	1.772449	0.354489705
9	2.1	52.164	17.09524	9	2.8388	0.315422217
13	0.7	17.388	51.28571	13	3.937412	0.302877865
17	0.3	7.452	119.6667	17	4.78471	0.281453535
Batch II						
1.5	39.8	988.632	1	0	0	****
3	10.1	250.884	3.940594	3	1.371331	0.457110496
6	3.2	79.488	12.4375	6	2.520716	0.42011935
9	1.7	42.228	23.41176	9	3.153239	0.350359851
12	0.7	17.388	56.85714	12	4.040542	0.336711821
15	0.3	7.452	132.6667	15	4.88784	0.325855981

Temperature dependency of rate equation:
The Arrhenius equation is given by,

$$k = k_o e^{\frac{-E}{RT}}$$

k at 67°C = 0.119 Per Hour
k at 80°C = 0.346 Per Hour
Substituting these values,

$$\frac{k_1}{K_2} = e^{(\frac{E}{R}(\frac{1}{T_1}-\frac{1}{T_2}))}$$

$$\ln(\frac{k_1}{K_2}) = \frac{E}{R}(\frac{1}{T_1}-\frac{1}{T_2})$$

$$\ln(0.119) = -2.129$$

$$\ln(\frac{0.119}{0.346}) = \frac{E}{R}(\frac{1}{67}-\frac{1}{80})$$

or

$$\frac{E}{R} = -440.062$$

$$\ln(k) = -2.129 + 440.0623(\frac{1}{67}-\frac{1}{T})$$

Using this equation, the other rate constants at other temperatures were calculated and are given in table below.

Table 7: Rate constants at various temperatures

Temperature(°C)	Rate constant (Per Hour)
67 °C	0.119
85 °C	0.478
97 °C	0.907

SELECTION OF CONSTRAINTS

The total TBA time cycle cannot exceed 8 hours, and the reaction has to be 99.9% complete within this time period. Thus these two were taken as the constraints. The constraints are tabulated below.

Table 8: Constraint table

Parameter	Max/Min value	Basis of calculation
Final conversion	0.1% (minimum)	K value calculated at 67°C, 85°C, 97°C
Total maintaining time	8 Hrs (maximum)	***

OPTIMIZATION PROCESS

The problem of TBA time optimization can thus be written as,

Maximize

Yield = $-0.044658(\mathrm{TWAT})^3+10.7839(\mathrm{TWAT})^2-871.459(\mathrm{TWAT})+24649.9$

Subject to the constraints

$$t_1 + t_2 + t_3 = 8$$

$$e^{-(0.119\,t_1 + 0.478\,t_2 + 0.907\,t_3)} \le 0.1$$

$$\frac{(67 * t_1 + 85 * t_2 + 97 * t_3)}{(t_1 + t_2 + t_3)} = TWAT$$

$$t_1 \ge 0$$

$$t_2 \ge 0$$

$$t_2 \ge 0$$

This is a non-linear program with four variables, two equality constraints and five inequality constraints. (Note that is has not been converted to the standard form)

RESULTS AND DISCUSSION

The following methods were used for optimization,

1. LINGO software
2. Microsoft excel solver
3. TABU search with extended neighborhood range (TSINR)

The values returned by the three methods are:

Table 9: Comparison of values returned by different optimizers

Optimization Method	Time (Hours)			2CB Yield (Kgs)
	67°C	85°C	97°C	
Original Value	1.5	3.0	3.5	1050
LINGO	6 Hours 17 Minutes	0 Hours	1 Hour 43 Minutes	1123.57
Excel Solver	6 Hours 17 Minutes	0 Hours	1 Hour 43 Minutes	1123.57
TSINR	6 Hours 17 Minutes	0 Hours	1 Hour 43 Minutes	1123.57

From table it is evident that all the optimization methods converged to the same global optimum. The constraint values are given by,

Table 10:Constraint table

Constraint	Original value	Derived from optimized value
Final conversion	0.2%	0.2 %
Total reaction time	8 Hrs	8 Hrs

SAVINGS

Neglecting the energy savings, the total savings per annum is calculated as follows.

Yield improvement per batch of 2CB = 73.57 Kgs
Average raw material cost of 2CB = 3.41 USD
Average number of batches of 2CB per month = 200

Thus savings per year assuming 11 month year = 551922 USD

Hence there could be monetary savings of about 551922 USD per year if the results were implemented.

INITIAL COST AND CAPITAL EXPENDITURE

There is absolutely NO EXPENDITURE involved in implementing the suggestions. The process merely involves changing the duration of temperature maintaining as suggested by the optimizer. No purchase of costly machinery or equipment is necessary. The same procedure can be tried out on a trial and error basis in the plant.

But this would involve much time and may seriously affect the yields if the results were negative. This optimization as done in the computer removes all risks and provides with a fair degree of flexibility for the process. The optimization program could predict with good accuracy the different parameters provided the assumed model is rigorous enough.

PROBLEM DEFINITION: 2CB BATCH CLEANING

This is another case study where the concept of heuristic model is applied. We follow the same guidelines as envisaged in previous chapters for the application of heuristic model.

STEP 1-SELECTION OF PROCESS TO BE OPTIMIZED

The process selected is the cleaning of 2CB reactors. Unlike the previous example, there are no chemical reactions involved in here. The 2CB reaction is done in SS316L vessels with TBAC (Tetra Chloro Butyric Acid) and IB (Iso Butylene) as reactants and hexane as solvent (TBAC is produced by the chlorination of TBA). TEA (Tri ethylamine) is also a reactant, which removes the HCl, produced as by-product.

A mixture of IB and hexane is taken in the reaction vessel. The quantity is dependent on the pressure developed inside the reactor since IB quantity cannot easily be quantized. Fixed quantities of TEA and TBAC are fed over a fixed time period. After the reaction is over the excess of Hexane and IB are vented off and recovered by scrubbing in chilled hexane (this mixture is used for the next reaction). Batch size is expressed as quantity of TBAC fed.

REASON FOR OPTIMIZATION

2CB reaction usually produces a tarry waste, which is found to reduce the reaction yield. There are no direct methods to remove this waste, which sticks to the vessel walls and impeller shaft. The usual procedure is after completing a certain number of batches, the reactor manhole is opened and sprayed with a solvent (Ethylene Dichloride - in this case) and remove the waste. But this process takes up time even though it increases reaction yield. Hence not all batches can be cleaned.

In plant we have fixed that 1 in every 5 batch will be cleaned. This batch is denoted as CL (for CLeaning) and the forth coming batches as NC1 (NonCleaning 1) NC2 (NonCleaning 2) depending on it’s precedence after the CL batch. The selection of this number (‘5’ in this case) is extremely difficult and hence we follow a method based on intuition rather than real optimization. Such a situation caters for a better balance between yield and time cycle. This study tries to mathematically find if this is the optimum value for 2CB batch cleaning frequency.

STEP 2 - COLLECTION OF RELEVANT PLANT DATA

The data obtained from plant for the month of March, 2003 for 6 kilomole batches is tabulated in table below.

Table 11: Different types of 2CB batches and corresponding average yield

Type of batch	Yield in Kgs	No. of batches
NC1	1109	38
NC2	1107	39
NC3	1100	38
NC4	1095	39
CL	1113	39

Thus for all types of batches this trend of decreasing yield is visible.

SCOPE OF OPTIMIZATION

This optimization does not envisage any process modification or change. It only tries to find out how we can arrive at a better system by optimum usage of resources. Instead of doing all this, if we could make an arrangement to clean the reactor after every batch with minimum down time, then that, no doubt will be a better option. But the method envisaged here involves no capital investment at all.

STEP 3 - SELECTION OF HEURISTIC MODEL

BASIS: One month of operation of four 2CB reactors.

The following terms need to be defined for optimization:

N_n = Number of non-cleaning batches.
Y_n = yield of non-cleaning batch.
N_c = Number of cleaning batches.
Y_c = yield of cleaning batch.
T_n = Time cycle for non cleaning batch
T_c = Time cycle for cleaning batch

The strategy here is to develop a heuristic model for total production for one month in terms of the batch cleaning frequency. Since production is not a direct function of frequency of cleaning, some mathematical manipulation will be required to arrive at the required model. Production is a function of number of batches and yield per batch.

$$\text{Production} = P = N \times Y \qquad (1)$$

Here N is the number of batches and Y is the yield per batch

Since we have both cleaning and non cleaning batches, the total production will be spilt between the two

$$P = N_nY_n + N_cY_c \qquad (2)$$

We know that non-cleaning batch is not a single one, but a combination of 4 non cleaning batches. Hence, the yield for a non-cleaning batch also will be a variable one. Time cycle, however remains the same.

The relation between cleaning and non-cleaning batches is given as,

$$N_n = (x - 1)N_c \qquad (3)$$

where x = 1,2,3,. . . no of cleanings.

Substituting equation 7.3, we get,

$$P = N_c\,(Y_n\,(x - 1) + Y_c) \qquad (4)$$

A similar treatment when applied to time gives equation 5

$$T_t = \text{Total time} = T_n N_n + T_c N_c \quad (5)$$

But total time, $T_t = 24 \times 30 \times 4 = 2880$ Hours
for a 30 day month and 4 reactors.

Substituting equation 4 and equation 3 in equation 5 and, we get

$$\text{Total time} = T_t = N_c\,(T_n\,(x - 1) + T_c) \quad (6)$$

Plant data show that a cleaning batch takes 16.5 hours average to complete and a non-cleaning batch takes 14.5 hours.

Substituting these values,

$$N_c\,(14.5(x - 1) + 16.5) = 2880 \text{ hours} \quad (7)$$

In addition, we have

$$N_c\,(Y_n\,(x - 1) + Y_c) = P \text{ Kgs} \quad (8)$$

Equation 8/ Equation 7

$$P = 2880 \frac{(Y_n(x-1) + Y_c)}{(14.5(x-1) + 16.5)} \quad (9)$$

Equation 7.9 is the heuristic model for 2CB batch cleaning frequency. It is evident that the model is a function of total time, yield per batch as well as batch cleaning frequency denoted by x.

STEP 4 - FITTING HEURISTIC MODEL TO AN EQUATION

The decrease in yield of 2CB batch is due to deposition of tarry materials and need not follow a fixed pattern. But we try to plot the data of the particular month so as to check if it follows a trend. The comparison of linear,quadratic and cubic fits are given in table 7.2,

Table 12: Comparison of data fits to plant data

Curve fit	Standard deviation
Linear	0.9698
Quadratic	0.9866
Cubic	0.9866

The linear fit which gives the least stadard deviation is selected. The curve-fit equation is

$$Y = 1118.5 - 4.5x \quad (10)$$

The physical meaning of equation 10 is that for every non-cleaning, the yield decreases by 4.5 kilograms. Substituting equation 10 in equation 9 gives

$$P = 2880\frac{((1118.5 - 4.5x)(x-1) + 1118.5)}{(14.5(x-1) + 16.5)} \tag{11}$$

STEP 5 - SELECTION OF CONSTRAINTS

The only constraint in the problem is that x should have a positive value. Though this seems surprising, it is to be noted that time constraint has been incorporated to the final heuristic model.

STEP 6 - INPUT TO OPTIMIZER

The problem of 2CB batch cleaning frequency optimization can thus be written as,

Maximize

$$P = 2880\frac{((1118.5 - 4.5x)(x-1) + 1118.5)}{(14.5(x-1) + 16.5)}$$

Subject to the constraints

$x > 0$

The equation 7.11 can be put into any optimizer and the value evaluated. But this equation is single variable and hence can be optimized by just substituting the values of x from 0 onwards.

The tabulated value is given in table

Table 13: Cleaning frequency and corresponding yields

X	P
1	195229.09
2	206969.80
3	210657.75
4	212131.20
5	212683.16
6	212764.04
7	212571.82
8	212207.18
9	211726.73
10	211164.73
11	210543.15

i.e. the peak production occurs at x = 5 or we have to clean once in every 5 batches.

RESULT

As practiced in the plant the reactor cleaning after every five batches is found to be mathematically the optimum value provided the assumptions made are entirely true. We have assumed that the decrease in yield per non-cleaning of batch is in a mathematical order and particularly a linear one. The value of x = 5 as derived here is the optima for the given month where the yield values follow a particular trend. When implemented practically, a better option will be a continuous optimization whereby we fit the curve after a fixed interval of time (say 5 days) and change the cleaning frequency as per this value.

CONCLUSIONS

The heuristic model was applied to the same production stage in the manufacture of Cypermethric Acid Chloride in two independent instances. While in the first case the objective was to optimize the reaction time and temperature,in the second case it was to check the optimality of cleaning of reactors. Optimized results were obtained in both the cases. Based on this,the advantages and disadvantages of the heuristic model based optimization process can be given as follows,

ADVANTAGES

The following are the advantages of the method,

1. The method is completely independent of the actual reason for the existence of constraints. Example: In example I the actual reason for the relationship between yield, temperature and time may be anything simple or complex. But the heuristic model does not have to take these into consideration.
2. The method requires no complicated derivations or mathematical modeling.
3. The method can be done with the least number of data points. Since the method is heuristics based, lesser number of data points actually works in favor in that it avoids the use of complicated models.
4. Any optimizer can be used for the final process optimization and given the optimizer gives global optima, the values have to be same. The number of iterations taken by the optimizer will depend on the efficiency of the algorithm used.
5. The method can be applied to both single and multi variable processes

DISADVANTAGES

The following are the drawbacks of the system:

1. The accuracy of the method will depend on the rigorousness of the heuristic model.
2. No generalized rule can be stated for the selection of heuristic models.

It can be concluded that heuristic model is any relationship between the given process parameters which is:

1. Approximate
2. Appropriate

The model is appropriate in that it represents a the trend shown by process variables. It is also approximate in that it is not a derived considering all the dependencies between the variables under consideration.

SCOPE FOR FURTHER WORK

The following things could be tried out as an extension to this work,

1. Try out the optimized parameters in plant.
2. Extend the method to continuous processes.
3. Extend the method to other manufacturing processes.

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