OPTIMIZATION MODEL FOR PRODUCTION AND SCHEDULING OF CATALYST REPLACEMENT IN A PROCESS WITH DECAYING PERFORMANCE

Martin Houze, Nikola Juhasz (1) and Ignacio E. Grossmann
Department of Chemical Engineering, Carnegie Mellon University
Pittsburgh, PA15213, USA (1) ATOFINA Chemicals, Inc

Abstract

This paper first describes an empirical model to characterize the deactivation of a catalyst used in the production of a specialty chemical based on actual plant data. This model is then used in a novel multiperiod MINLP optimization formulation that incorporates the empirical model in order to determine the optimal catalyst replacement policy and meet time varying product demand.

Keywords: Catalyst management, catalyst deactivation, MINLP, planning, scheduling

Introduction

The operation of catalytic processes with decaying performance involves a challenging modeling and optimization problem. As the catalyst activity decreases over time, plant shutdowns for catalyst changeovers must be planned to restore the plant performance. When optimizing the plant profit, the trade-off is between the high production rates achieved from maintaining frequently renewed, high-functioning catalyst loads and the maintenance costs and loss in production due to shutdowns.

Catalyst deactivation has received attention with kinetic studies at the reactor level (Gutierrez-Ortiz, 1984) and pilot plant level. Regarding plant optimization, the problem of scheduling multiple feeds on parallel units with decaying performance has been addressed by Jain and Grossmann (1998). This work considered the case where the customer demand is constant on an infinite time horizon. The optimization of catalyst management policy for oxo processes has been addressed, using a non-linear programming (NLP) strategy by Lang, Biegler, Maier and Majewski (2000).

In this paper, an empirical model is first formulated based on data collected from three catalyst loads run at an industrial plant over the past few years, and with key process parameters known to influence productivity and catalyst deactivation. The parameters of the model are determined with nonlinear regression by least squares minimization. As will be shown, a reasonably good fit to the plant data can be obtained. The second element that is described in this paper is a multiperiod optimization model that maximizes the profit from the process based on the selection of the best operating policies over time given the model for decay in catalyst activity and production. The optimization model also ensures that seasonal customer demands and minimum inventory levels are met. Over a multi-year time horizon, three main decisions are to be made with this model: a) number of catalyst loads to be used; b) timing when the catalyst changeovers are to be scheduled; c) operational profiles on process parameters such as reactor temperature and flow through the reactor. A mixed integer nonlinear programming (MINLP) model, using the empirical model is formulated and solved for an actual industrial application.

Development of the empirical model

The reaction addressed in this paper is of the following form: A+B→C+D. C is the specialty chemical. Another compound X is injected in the reactor to prevent catalyst deactivation. Daily-averaged plant data on three different catalyst loads of approximately six months each is considered. The plot in Figure1 shows production data for the first catalyst load, as well as the model that was fit according to the following equation, Pday = f(T,P),

$$\mathrm{Pday} = K \times Act \times \exp\left(\frac{-Ea}{\mathrm{R} * \mathrm{T}}\right) \times \mathrm{F}^{nf} \times \mathrm{X}^{nx} \times \mathrm{B}^{nb} \times \mathrm{P}^{np} \qquad (1)$$

with R is the perfect gas constant and the following parameters were determined:

K: Coefficient (psig^{-1})
Ea: Activation energy ($\mathrm{J.mol}^{-1}$)
n_f: Flow exponent
n_x: exponent for the percentage ratio of X to C
n_b: exponent for the percentage ratio of B to C
Act: the activity of the catalyst

In Figure 1, the predictions follow the general profile of the observations. For confidentiality reasons, the units used are arbitrary.

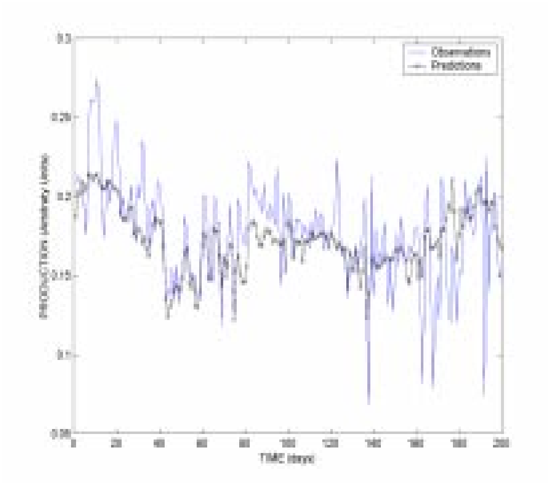

Figure 1. Predictions and Observations of Plant production

MINLP model

The formulation of the profit optimization model uses the following assumptions:

- The time to shut down the plant, remove the catalyst from the reactor and reload it with a fresh catalyst batch is estimated at one month.
- Monthly predictions over a two-year period for customer demand are considered.

The problem considered here is to determine how many catalyst loads should be used, when should the catalyst changeovers be scheduled and what are the best profiles for temperature and flow through the reactor. The basic idea is to use discrete time representation in which the changeout is considered on a monthly basis, but changes at the operating conditions are considered on a weekly basis.

For the sake of clarity of presentation, a time horizon of 2 years is considered and divided into monthly time periods. Between one and four catalysts may be scheduled in total (c=1,..4). Predictions of customer demand for each period are provided by a marketing study. The production of the plant may be optimized using two parameters: temperature and loop flow through the reactor. To comply with the plant policy, the inventory is to be kept over a minimum level. The following is the nomenclature for the model formulation.

Indices:

i: denotes the months (from 1 to 25)
w: denotes the weeks (from 1 to 4)
c: denotes the catalysts

Note: the 25th period is defined as end condition. By convention, when a catalyst is not used, its time of disposal is set to Td_c=24 and the downtime occurs during the 25th period.

Parameters:

Vol: Catalyst mass (lb)
Cc: Catalyst cost, (Million $/lb)
VM: Variable Margin or net profit on the final product ($/lb)
Cs: Cost of storing a pound of product ($/lb)
Dmd_i: Prediction for customer demand on month i (million $)
$Stock_0$: Initial stock level (Million lb)
LowestStock: Lowest Stock level (Million lb)
T_o : Starting temperature (F)
R1 Upper bound on the temperature increase rate (F/month)
BM, BM2, BM3, BM4, BM5, BM6, BM7 are big-M parameters for conditional constraints.

Binary variables:

x_c: indicates whether catalyst c is used or not
$y_{i,c}$: indicates when the catalyst c is changed, $y_{i,c}$=1 means catalyst c is changed over period i
$z_{i,c}$: indicates when catalyst c is used, $z_{i,c}$=1means catalyst c is used over period i
$a_{i,c}$: binary variable used for defining $z_{i,c}$
$b_{i,c}$: binary variable used for defining $z_{i,c}$

Continuous variables:

P_i: Production obtained in period i (nil when downtime occurs) (Million lb)
$Pmth_{i,c}$: Monthly production, is used to compute the cumulative production and the lost production when a downtime occurs. (Million lb)
$Penalty_{i,c}$: Penalty related to a downtime, is computed by calculating the lost production (Million $)
$CP_{i,w,c}$: Cumulative production (Million lb)
$Stock_i$: Stocklevel in period i (Million lb)
$Sales_i$: Sales achieved in period i (Million lb)
Ben:Profit for the total time horizon (Million $)
$T_{i,c}$: Reactor temperature in period i
F_i: Flow through the reactor in period i
Td_c: Time of disposal of catalyst c, beginning of the downtime following the use of catalyst c (Month)
$Pweek_{i,w,c}$: Production on week w, month i, with catalyst c (Million $)
$UDmd_i$: Unmet demand on month i (Million $)
X: Mass ratio of X to C

Figure 2 shows the definition of the major variables for the problem. Td_c is the time for the beginning of the downtime when catalyst c is removed. The binary variable $z_{i,c}$ is equal to 1 when catalyst c is used or being replaced, and zero otherwise.

The following equation is the objective function to be maximized.

$$Ben = \mathrm{VM} \times \sum_{1}^{24} Sales_i - \mathrm{Cc} \times \sum_{1}^{4} x_c - \mathrm{VM} \times \sum_{1}^{24} UDmd_i - \mathrm{VM} \times \sum_{1}^{24}\sum_{1}^{4} Penalty_{i,c} - \frac{\mathrm{Cs} \times \sum_{1}^{24} Stock_i}{24} \quad (2)$$

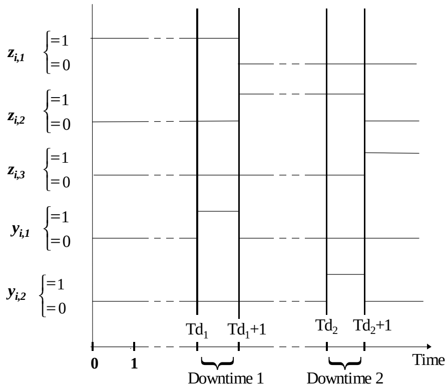

Figure 2: Representation of the problem

The following equation defines the time of disposal of catalyst c.

$$Td_c = \sum_{i=1}^{i=24} (i-1) \times y_{i,c} \quad (3)$$

The equations below calculate the monthly production. When the catalyst c is used in period i, then the production is computed using the empirical formula presented in section:

$$\left.\begin{aligned} Pweek_{i,w,c} &\le f(T_{i,c}, P, CP_{i,w,c}) * 7 + \mathrm{BM2} * (1 - z_{i,c}) \\ Pweek_{i,w,c} &\ge f(T_{i,c}, P, CP_{i,w,c}) * 7 - \mathrm{BM2} * (1 - z_{i,c}) \end{aligned}\right\} \forall i \ne 25 \quad (4)$$

The equations below ensure that the production for catalyst c in period i is nil when the catalyst is not used:

$$\left.\begin{aligned} Pweek_{i,w,c} &\le 0 + \mathrm{BM2} \times z_{i,c} \\ Pweek_{i,w,c} &\ge 0 - \mathrm{BM2} \times z_{i,c} \end{aligned}\right\} \forall i \ne 25 \quad (5)$$

The following equality calculates the monthly production.

$$Pmth_{i,c} = \sum_{w=0}^{w=3} Pweek_{i,w,c} \quad \forall i \ne 25 \quad (6)$$

The following inequalities compute the cumulative production every week w:

$$\begin{aligned} CP_{i,w,c} &\le \sum\nolimits_{i=1}^{i} Pmth_{i,c} + \sum\nolimits_{w=0}^{w} Pweek_{i,w,c} + \mathrm{BM} * (1 - z_{i,c}) \\ CP_{i,w,c} &\ge \sum\nolimits_{i=1}^{i} Pmth_{i,c} + \sum\nolimits_{w=0}^{w} Pweek_{i,w,c} - \mathrm{BM} * (1 - z_{i,c}) \\ CP_{i,w,c} &\le 0 + BM * z_{i,c} \end{aligned} \quad (7)$$

The following equations are product balances for the inventories:

$$\begin{aligned} Stock_0 + P_i &= Sales_i + Stock_i \quad if\ i = 1 \\ Stock_{i-1} + P_i &= Sales_i + Stock_i \quad \forall i \ne 1 \ne 25 \end{aligned} \quad (8)$$

The following equation calculates the unmet demand:

$$UDmd_i = Dmd_i - Sales_i \ \forall i \ne 25 \quad (9)$$

The following inequality constrains the temperature increase rate to R1 F/month

$$T_{i+1,c} - T_{i,c} \le \mathrm{R1} + \mathrm{BM5} \times (1 - z_{i,c}) \ \forall i \ne 25 \quad (10)$$

The following inequality is relaxed from the equality that computes the monthly production as the sum of the Pmth:

$$P_i \le \sum_{c=1}^{c=4} Pmth_{i,c} \ \forall i \ne 25 \quad (11)$$

The following inequality ensures that the monthly production is nil when a downtime occurs:

$$P_i \le \mathrm{BM6} \times (1 - y_{i,c}) \quad (12)$$

The next inequality is obtained by relaxing the equality that computes the downtime penalty as the lost production:

$$Penalty_i \ge Pmth_{i-1,c} - \mathrm{BM3} \times (1 - y_i) \ \forall i \ne 25 \quad (13)$$

The inequalities below ensure that the temperature used to compute the penalty (production that would have been achieved during a downtime) cannot be lower than T_0 F.

$$T_{i+1,c+1} \ge \mathrm{T_o} - \mathrm{BM5} \times (1 - y_{i,c}) \ \forall i \ne 25 \quad (14)$$

The following constraints define $z_{i,c}$ for the first catalyst:

If the period considered is before td_c+1, then $z_{i,c}$ equals 1.

$$i \le td_c + 1 + \mathrm{BM6} \times (1 - z_{i,c}) \quad if\ c = 1, \forall i \ne 25 \quad (15)$$

If the period considered is after td_c +2, then $z_{i,c}$ equals 0.

$$i \ge td_c + 2 - BM6 \times z_{i,c} \quad if\ c = 1, \forall i \ne 25 \quad (16)$$

To define $z_{i,c}$ for the second and third catalyst, it is necessary to introduce the binary variables $a_{i,c}$ and $b_{i,c}$. The plot below shows how $a_{i,c}$ and $b_{i,c}$ shifts from 0 to 1.

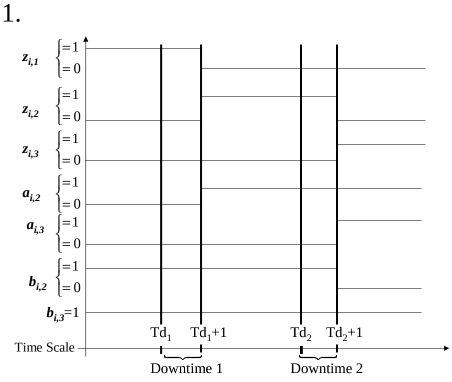

Figure 3. Definition of variable $z_{i,c}$, $a_{i,c}$ and $b_{i,c}$

The inequalities below define $z_{i,c}$ through $a_{i,c}$ and $b_{i,c}$ for the catalysts 2 and 3:

$$\left.\begin{array}{l} i \ge td_{c-1} + 2 - \mathrm{BM6}\times(1 - z_{i,c}) \\ i \le td_c + 1 + \mathrm{BM6}\times(1 - z_{i,c}) \\ i \le td_{c-1} + 1 + \mathrm{BM6}\times a_{i,c} \\ i \ge td_{c-1} + 2 - \mathrm{BM6}\times(1 - a_{i,c}) \\ i \le td_c + 1 + \mathrm{BM6}\times(1 - b_{i,c}) \\ i \ge td_c + 2 - \mathrm{BM6}\times b_{i,c} \end{array}\right\} \forall i \ne 25, \forall c \ne 1 \ne 4 \quad (17)$$

The following define $z_{i,c}$ for the fourth catalyst:

$$\left.\begin{array}{l} i \le td_{c-1} + 1 + \mathrm{BM6}\times z_{i,c} \\ i \ge td_{c-1} + 2 - \mathrm{BM6}\times(1 - z_{i,c}) \end{array}\right\} \forall i \ne 25, if\ c = 4 \quad (18)$$

To ensure that only one changeout occurs when a catalyst is replaced, the following must hold:

$$\sum_{i=1}^{i=24} y_{i,c} = x_{i,c} \quad (19)$$

The next constraints define the value of variable $x_{i,c}$ ($x_{i,c}$ equals 1 when td_c is lower than 24.)

$$\begin{array}{l} td_c \ge 24 - \mathrm{BM7}\times x_c \\ td_c \le 23 + \mathrm{BM7}\times(1 - x_c) \end{array} \quad (20)$$

To ensure that catalyst c+1 can only be used after catalyst c, the following inequality is imposed,

$$x_c \ge x_{c+1} \forall c \ne 4 \quad (21)$$

The following constraint ensures that only one catalyst can be used at a time,

$$\sum_{i=1}^{i=24} z_{i,c} \le 1 \quad (22)$$

while the following inequality ensures that a catalyst is only disposed once:

$$\sum_{i=1}^{i=24} y_{i,c} \le 1 \quad (23)$$

The following constraint ensures that when catalyst c is disposed of, a new catalyst c+1 is used. In other words, if catalyst c is used, then catalyst c is used too,

$$\sum_{i=1}^{i=24} z_{i,c} \ge x_c \quad (24)$$

The inequality below ensures that only one downtime happens over the same period,

$$\sum_{c=1}^{c=4} y_{i,c} \le 1 \quad (25)$$

while the constraint that sets the minimal catalyst age before disposal to five months is as follows,

$$\sum_{i=1}^{1=24} z_{i,c} \ge 5 \quad (26)$$

The model in (2)-(26) corresponds to a multiperiod MINLP that has been solved with the code DICOPT in GAMS (Viswanathan and Grossmann, 1990.)

Results

The proposed two-year time horizon model was successfully solved. A similar four-year time horizon model was also formulated and solved. As shown in Table 1, the four-year time horizon model becomes large and more difficult to solve.

	2-year horizon time model	4-year horizon time model
Discrete Variables	299	587
Variables	1503	2943
Equations	3960	8576
Solution time	132 CPUsec	1440 CPUsec

Table 1: Computational statistics

The production and sales for the two-year problem are plotted in Figure 4.

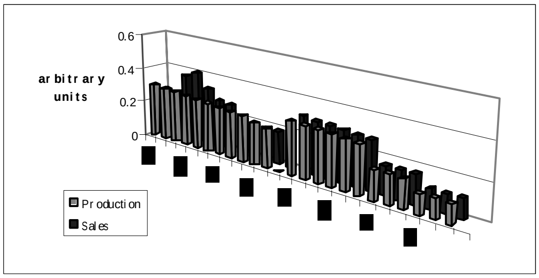

Figure 4. Production and Sales profile

As shown in Figure 4 the downtime is scheduled in December of the first year, during the lower demand season. In addition, the order of magnitude for the production and sales is close to the one achieved at the plant. Based on these observations, we think that the fidelity of the model is acceptable.

When testing the sensitivity of the 2-year horizon time model to variations in parameters, it was found that the profit is most sensitive to a variation of the variable margin and least sensitive to a variation of the cost of the catalyst. In all cases except one, the downtime occurs in month 12 of the first year, which is consistent with the demand forecast.

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