

International Symposium on Advanced Control of Chemical Processes Gramado, Brazil – April 2-5, 2006



# MULTIPERIOD OPTIMIZATION MODEL FOR SYNTHESIS, DESIGN, AND OPERATION OF NON-CONTINUOUS PLANTS

Gabriela Corsano, Jorge M. Montagna, Pio A. Aguirre, and Oscar A. Iribarren

INGAR – Instituto de Desarrollo y Diseño Avellaneda 3657, S3002 GJC Santa Fe, Argentina

Abstract: In this paper, a general multiperiod nonlinear optimization model is presented, which incorporates synthesis, design, and operation, and takes into account the corresponding benefits and costs in each time period. The model is formulated as a non linear programming (NLP) model in which plant structure decisions are modeled in terms of a superstructure embedded in the overall model. This approach is novel since it involves new decision variables, integrates algebraic and differential equations, and solves a NLP problem even when discrete decisions are involved. The proposed model is applied to a Brandy production plant with high detail level in the operations description. The optimal solution is found and different tradeoffs between process and design variables are assessed. *Copyright* © 2005 IFAC

Keywords: Structured Programming, Synthesis, Design, Process Models, Optimization, Nonlinear Programming

# 1. INTRODUCTION

Multiperiod plants are process plants where costs, demands and resources typically vary from period to period due to market or seasonal changes. Models for multiperiod optimization have an objective, e.g. maximize total profit or minimize cost, which is subjected to constraints that represent mass balances, process performance equations or design equations. Some constraints can be valid for all periods or for an individual period. These models typically involve both continuous and discrete variables, and consequently most mathematical formulations for this problem result in a mixed integer nonlinear programming (MINLP) model (Voudouris and Grossmann, 1992; Paules, and Floudas, 1992; Varvarezos et. al. 1992; Van den Heever and Grossmann, 1999).

MINLP problems are usually solved through methodologies that successively solve Mixed Integer Linear (MILP) approximations to the model and NLP problems for fixed configurations, i.e. certain decisions as regards the value of binary variables (Viswanathan and Grossmann, 1990). For the case of a non-convex problem, the drawback of this mechanism is the fact that successive linearizations usually cut part of the feasible region. In this way, some solutions to the problem are lost (Grossmann, 2002). In addition, many solutions of plant configurations, which are found through MILP, correspond to non-feasible structures, which are not suitable for meeting production requirements.

In order to overcome the aforementioned difficulties, a general nonlinear programming (NLP) model is proposed in this paper, where plant structure decisions are simultaneously considered with the process and design variables. In this way, both discrete variables and the complexity of solving a MINLP are avoided. The structured plant is obtained for all periods, and therefore different tradeoffs between process and design variables are analyzed in each time period.

A study case that considers the seasonal production of Brandy is presented in this work. The proposed model presents a high detail level that is rarely found in the literature. The mass balances for some units in each period are given in terms of dynamic equations written as algebraic equations and included in the overall model. Design equations require process performance variables, operative conditions, and several raw materials and energy resources to be taken into account in order to obtain a real scenario for this process production. The paper is organized as follows. The next section presents the problem description. In Section 3, the general formulation proposed for the optimal synthesis, design and operation of a multiperiod plant is formulated. The Brandy process production is described in Section 4; and the results of its model optimization is presented in Section 5. Some comments and results analysis are also presented in this last section. Finally, conclusions are presented in Section 6.

#### 2. PROBLEM STATEMENT

A non-continuous plant involves two types of units: batch  $(j = 1, ..., N_j)$  and semicontinuous  $(k = 1, ..., N_k)$ . In addition, the process considered in this paper is monoproduct, i.e., only one product is produced. For each time period t (t = 1, ..., T), the product is manufactured in each unit. In this model, the plant structure is the same for all periods. The number of periods, the total time horizon HT and the time horizon for each period  $H_t$  is a data problem. For some batch stages, the number of units in series is unknown beforehand and the stage configuration is decided including the superstructure model presented by Corsano et al. (2004) in the overall model. In this way, the use of binary variables is avoided.

The plant receives raw materials and energy resources r ( $r = 1, ..., N_r$ ) of another plant (mother plant) that seasonally produces them within the same industrial complex. Therefore, in some time periods, the non-continuous plant must buy material and energy resources from another industrial complex. Resources obtained from the mother plant have no cost.

Batch blending, batch splitting and recycles are allowed as novel components for this type of models, decisions taken in this work as optimization variables. The transfer policy adopted between batch stages is Zero-Wait (ZW).

The objective is to maximize the total benefit considering incomes from product sales and operative and investment costs.

### 3. MATHEMATICAL FORMULATION

Given *T* periods of time over the horizon time *HT*, the model considers:

*Objective Function:* Maximization of annualized net profits given by the total expecting selling price minus the investment and operative cost is considered

$$Max \sum_{t=1}^{T} p_t Nb_t B_t - \left(\sum_{j=1}^{N_j} \alpha_j V_j^{\beta_j} + \sum_{k=1}^{N_k} \alpha_k V_k^{\beta_k} + \sum_{t=1}^{T} \sum_{r=1}^{N_r} c_{rt} F_{rt}^{trans} + Res\right)$$
(1)

where  $p_t$  is the expected net profit in period t,  $Nb_t$  the number of batches produced in period t,  $B_t$  the product batch size in period t, V are the batch (j) and semicontinuous (k) unit size,  $F_{rt}^{trans}$  is the amount of resource r transported from a plant other than mother plant in period t and  $c_{rt}$  is its cost that considers supply and transportation costs.  $\alpha$  and  $\beta$  are the cost coefficients and *Res* the disposal cost that varies according to the effluent.

*Mass balances at each unit of the plant:* some material balances are given by differential equations like

$$\frac{dC_{xjt}}{d\tau} = g(\tau, x, t) \tag{2}$$

which are discretized and included in the global model as algebraic equations. We adopt the trapezoidal method to discretize the differential equations. The performance of this method for this kind of models was analyzed in Corsano et al. (2004). The difference finite equations according to the trapezoidal method are

$$C_{xjt}^{n+1} = C_{xjt}^{n} + \frac{h}{2} \left( g(\tau_n, C_{xjt}^n) + g(\tau_{n+1}, C_{xjt}^{n+1}) \right)$$
(3)

where  $C_{xjt}$  is the concentration of component x (biomass, substrate, product, etc.), at stage j in period t.  $\tau$  represents the time variable and  $h \ge 0$  defines the discretization grid points by  $\tau_n = \tau_0 + nh$  and  $n \ge 0$ .

*Mass balances between units of the same plant:* blending of batches is considered in this model, so a batch unit size depends on the previous unit batch size and the batch size of the feeding to this unit. The model considers *global material balances*:

$$VS_{jt} = \sum_{r=1}^{N_r} f_{rjt} + VS_{j-1,t}$$
(4)

and component material balances:

$$VS_{tj}C_{xjt}^{ini} = \sum_{r=1}^{N_r} C_{xjt}^r f_{rjt} + C_{x,j-1,t}^{fin} VS_{j-1,t}$$
(5)

where superscripts *ini* and *fin* represent the initial and final concentration respectively and  $VS_{jt}$  represent the batch volume at stage *j* in period *t*.  $f_{jrjt}$  is the amount

of *r* consumed at stage *j* in period *t*; and  $C_x^r$  represent the concentration of *x* in *r*.

Interconnection constraints between mother plant and multiperiod plant:

$$F_{rt} + F_{rt}^{trans} \ge \sum_{j=1}^{N_j} \frac{f_{rjt}}{CT_t} + \sum_{k=1}^{N_k} \frac{f_{rkt}}{CT_t} \text{ for each } r \quad (6)$$

where  $F_{rt}$  is the amount of resource *r* produced by the mother plant in period *t* and *CT* indicates the plant cycle time.  $F_{rt}^{trans}$  represents the amount of resource *r* that must be transported from another plant in period *t*. Resources obtained from the mother plant have no cost, and as a consequence, only transported resources costs are considered in the objective function.

Design equations: for each batch units

$$V_j \ge S_j B_t$$
 for each period  $t$  (7)

and semicontinuous units

$$V_k \ge S_k \frac{B_t}{\theta_{kt}}$$
 for each period  $t$  (8)

where *B* is the product batch size (kg); *S* represents size or duty factor of batch and semicontinuous units which depends on process variables; and  $\theta_{kt}$  is the processing time of unit *k* in period *t*. Note that these constraints are in " $\geq$ " form because some units can be sub-occupied in some period.

*Constraints of production rate of the plant:* 

$$\frac{Nb_t B_t}{CT_t} = Q_t \tag{9}$$

$$Q_t^{\min} \le Q_t \le Q_t^{\max} \tag{10}$$

where  $Q_t$  is the production rate in period *t* which is bounded by  $Q_t^{\min}$  and  $Q_t^{\max}$ ; and  $CT_t$  is the cycle time of the plant on period *t*.

*Timing constraints:* as the plant produces only one product, the ZW transfer policy indicates that

$$CT_t \ge T_{it}$$
 for all *j* batch units (11)

$$CT_t \ge \theta_{kt}$$
 for all k semicontinuous unit (12)

where

$$T_{jt} = \theta_{k't} + t_{jt} + \theta_{k''t} \tag{13}$$

 $T_{ji}$  represents the time for which batch unit *j* will be occupied, which contemplates the material loading  $(\theta_{k'i})$  and unloading  $(\theta_{k''i})$  time if this unit is located between semicontinuous units.  $t_{ji}$  is the processing time of unit *j*. It is worth noting that in this approach, variables  $t_{ij}$  and  $\theta_{ik'}$  are assumed to be involved in detailed submodels, some of them written as differential equations and included in the actual model.

The product in each period must be produced within the period horizon time, so

$$Nb_t CT_t \le H_t$$
 for each  $t = 1, ..., T$  (14)

and

$$\sum_{t=1}^{T} H_t \le HT \tag{15}$$

# 4. STUDY CASE: A BRANDY PRODUCTION PLANT

A Brandy production plant that receives material and energy resources from a neighboring Sugar plant is considered. Besides producing this alcohol, the Brandy plant generates a non-distilled remainder called vinasses or distillery broth that represents another contribution of sugaring substrate for fermentations stages. Four stages for Brandy production are considered: biomass fermentation, alcohol fermentation, centrifugation and distillation. The main objective of the first stage is biomass production. This stage operates in batch form and it is fed with molasses and filter juices from the sugar plant, vinasses, and water. The first biomass fermentor is fed with a broth containing biomass prepared in laboratory: the inoculums. At this stage, large amounts of air are supplied. The alcohol fermentor is also a batch item and it is fed with the product of biomass fermentors, molasses, filter juices, vinasses, and water. Brandy production occurs at this stage without air supply. The fermented broth is centrifuged in a disk stack centrifuge that operates in a semicontinuous mode. The objective of this stage is to separate the biomass from the liquid that contains the brandy. The solids can be recycled to a Yeast production plant. In this work, yeast production is not considered. The last stage of the process is the batch distillation. The batch distiller model is a combination of two batch items, namely the distiller feed vessel and the distillate tank, and three semicontinuous items: the heating surface to evaporate, the cooling area to condense the steam and the column itself. An analytical model presented by Zamar et al. (1998) for batch distillation is adopted. This model relates both the minimum and operational reflux values as well as the minimum and operational number of stages.

For biomass and alcohol fermentations, the superstructure model presented by Corsano et al. (2004) is included in the overall model in order to find the optimal synthesis and design of these stages. In this paper, only duplication of units in series is considered.

The sugar plant produces molasses, filter juices, electricity and vapor that are used for Brandy production. Molasses and filter juices serve as sugaring substrates for biomass and alcohol fermentations. In addition, water and vinasses are added to the fermentation feed. The electricity generated in the sugar plant is used in the centrifuge of the plant, whereas fermentors and the distillation column consume the steams.

For the Sugar plant, two seasons are distinguished: harvest and no-harvest date. During the harvest date, the Sugar plant provides molasses, filter juices, electricity, and vapor to the Brandy plant. In addition, if necessary, molasses, vapor, and electricity can be imported from other plants, allocating operative costs to the total annual cost due to the purchase and transportation of these products.

During the no-harvest date, vapor and electricity are imported from other power stations. The molasses that are not consumed during the harvest date can be stored, while filter juices cannot, since they are degraded in a short time. The model considers an additional cost for molasses inventory and for importations and transportation of electricity and vapor. Again, if needed, molasses can be imported from another complex. Figure 1 shows the flowsheet for Brandy production plant.



Fig. 1. Flowsheet for Brandy Production Plant integrated to a Sugar plant

The produced vinasses have a substrate concentration variable that depends on the processing time of the last alcohol fermentor in the series, that is, there is a tradeoff between processing time of this unit and the substrate concentration of the vinasses. A longer processing time implies a smaller substrate concentration because the substrate is consumed in fermentation stages. Unused vinasses are discarded and a disposal cost is added in the objective function (*Res* in equation (1)).

For this model, we consider a total time horizon of 7500 hours divided in two periods: harvest with 3000 hours and no-harvest with 4500 hours. Table 1 shows the adopted cost for material and energy resources imported in each period and the amount produced for the Sugar plant in harvest period. Production rates for both periods are lower and upper bounded by  $0.5 \text{ t h}^{-1}$  and 2 t h<sup>-1</sup> respectively.

# 5. RESULTS AND ANALYSIS

The model was implemented and solved in GAMS (Brooke et al., 1998) in a Pentium IV, 1.60 Ghz. The code CONOPT2 was employed for solving the NLP problems. The number of equations and variables is about 3000 and 3200 and the CPU time needed for resolution is 340 sec.

Table 1.	Material	and	energy	imported	resources cost

	Harvest Date	No- Harvest	Sugar plant production
	1	Date	production
Molasses	$10 \ \text{s} \ \text{t}^{-1}$	35 \$ t <sup>-1</sup>	36 t h <sup>-1</sup>
Stored		<b>σ φ 4</b> -1	
molasses	- ,	531	- ,
Vapor	$3.53 \ \text{s} \ \text{t}^{-1}$	8.5 \$ t <sup>-1</sup>	4.6 t h <sup>-1</sup>
Electricity	0.02 \$ kwh <sup>-1</sup>	0.04 \$ kwh <sup>-1</sup>	260 kwh
Inoculums	1 \$ kg <sup>-1</sup>	1 \$ kg <sup>-1</sup>	-
Water	$0.05 \ \text{s} \ \text{t}^{-1}$	0.05 \$ t <sup>-1</sup>	-

The optimal solution obtained for the Brandy production plant considering two different periods of time consists of a plant with one biomass fermentor and three alcohol fermentors in series. Table 2 shows the optimal design variables and the processing time of each unit in each period.

The cycle time of the plant is equal to 11.2 h for the harvest date and 13.7 h for no-harvest date, and the number of batches at each period is 268 and 328 respectively. Production rate in each period is equal to 2 t h<sup>-1</sup> (upper bound). Total profit is  $3575.8 \text{ s} \text{ h}^{-1}$ . Table 3 shows the resources used in each period and the resources bought in the no-harvest period. In harvest period, all resources used the in Brandy plant come from the Sugar plant. The table also shows the cost for the purchased resources.

As shown in Table 3, molasses used in the no-harvest period are the totally stored molasses, so that no molasses are imported from other sugar complexes. Water included in the table corresponds to the consumed water in fermentation stages, but its reported costs are the sum of the cost for water in fermentation and the cost for cooling water in distillation column.

 Table 2. Optimal design variables and processing

 times in each period

		Processing times	
	Unit	Harvest	No-
	Size	Date (h)	Harvest
			Date (h)
Biomass	81.9 m <sup>3</sup>	11.2	13.7
Fermentor			
Alcohol Ferm. 1	294 m <sup>3</sup>	11.2	13.7
Alcohol Ferm. 2	329 m <sup>3</sup>	8.8	12.1
Alcohol Ferm. 3	372.2 m <sup>3</sup>	8.8	4.11
Centrifuge	70.6 Kwh	2.3	9.4
Distillation		8.8	4.3
Stages Number	9		
Reflux Ratio	5.2		
Distillate Tank	$34.8 \text{ m}^3$		
Still Vessel	277.1 m <sup>3</sup>		
Condenser Area	117.6 m <sup>2</sup>		
Evaporator Area	69.6 m <sup>2</sup>		
Column	2.9 m <sup>2</sup>		

Table 3. Resources used in each period and costs

	Harvest Date	No- Harvest Date	Cost (\$ h <sup>-1</sup> )
Molasses	26.4 t h <sup>-1</sup>	9.6 t h <sup>-1</sup>	48.15
Vapor	2.12 t h <sup>-1</sup>	1.27 t h <sup>-1</sup>	10.8
Electricity	70.6 Kwh	11.1 Kwh	0.41
Inoculums	3.9 kg h <sup>-1</sup>	0.7 kg h <sup>-1</sup>	4.64
Water	$0.1 \text{ t} \text{ h}^{-1}$	0.02 t h <sup>-1</sup>	$17.3^{1}$
Vinasses	$6.3 \text{ m}^3 \text{ h}^{-1}$	$6.4 \text{ m}^3 \text{ h}^{-1}$	$3.62^{2}$

The optimal substrate concentration in vinasses is 2.1 g  $l^{-1}$  for harvest date (o period?) and 49 g  $l^{-1}$  in noharvest date. Having this substrate concentration variable allows a better performance in molasses utilization. Since molasses are more expensive in the no-harvest period, vinasses substrate concentration is increased in order to attain more concentrated blending to fermentation stages. In order to obtain a higher vinasses substrate concentration, fermentation stages have idle time due to the existing tradeoff between these two processing variables (as previously mentioned). Figure 2 shows the substrate concentration in each fermentor for both periods; and as it can be noted, the substrate in the last fermentor for no-harvest date is not totally consumed in order to attain higher substrate concentration in vinasses.



Fig. 2. Substrate concentration in fermentation stages of each period

Total produced vinasses in no-harvest period are recycled to fermentation stages, while about 30% of the produced vinasses in harvest time are discarded.

If more vinasses were used in fermentation stages, the unit sizes would be increased and therefore the investment cost of fermentation stages would be also increased. So, there is another trade-off between vinasses use and fermentation investment cost.

In no-harvest period, some units are sub-occupied. This means that the batch size is smaller than the unit size. This occurs with the three alcohol fermentors, where only about 65% of the units are used.

Simultaneously optimizing synthesis, design, and operation allows obtaining solutions that differ from those obtained in the usual industrial practice, and thus research in this direction is worth being explored. In general, these problems are dealt with by separate: first the plant configuration problem, then the sizing problem and last the operation and scheduling optimization. This leads to sub-optimal solutions. Therefore, simultaneous optimization enables obtaining more accurate solutions and analyzing the tradeoff between different process and design variables.

### 6. CONCLUSION

A general formulation for the simultaneous synthesis, design and operation for a non-continuous multiperiod plant was proposed and modeled as a NLP problem. Integration between units as well as variable feed blends, unit sizes and operation times were taken into account.

There are no previously published works dealing with simultaneous optimization of the plant structure, design and process variables for a multiperiod plant formulated as a NLP problem. The NLP formulation

<sup>&</sup>lt;sup>1</sup> Water cost includes distillation column cooling water and fermentation fresh water cost.

<sup>&</sup>lt;sup>2</sup> Vinasses cost represents the disposal vinasses cost.

avoids difficulties that arise with resolution methodologies of MINLP problems applied to non convex programs.

The model was applied to a Brandy production plant with two time periods: harvest and no-harvest. The optimal number of units in series of the fermentation stages was determined simultaneously with the optimal values of the process variables and the optimal sizing of the downstream stages.

A model with a high level of detail was presented. Operations have been represented through discretized differential equations that describe mass balances (in this case, mass balances of batch fermentors). Furthermore, constraints on feeds to each processing unit, recycles, and equations of interconnections between stages are considered. It is a level of detail that has been posed by few authors.

The model solution allowed analyzing different tradeoffs between process and design variables: the presence of idle times in the fermentation stages and vinasses substrate concentration, the vinasses disposal and the unit size of fermentation stages, molasses use and vinasses substrate concentration.

Duplication in series of biomass fermentors is an industrial practice, while duplication in series of alcohol production fermentors is not. And for the particular case of Brandy production from sugar plant residuals, vinasses recycles are rarely used. In our opinion, a strong point of this research report is that constructing a model for simultaneously optimizing the plant structure and process variables allowed envisaging that plant structures and process variables figures different from those of the current industrial practice may be worth exploring.

Furthermore, with the specific results presented in this work, this approach shows the capabilities of integrated formulations that simultaneously consider synthesis, design and operation decisions applied to a multiperiod context. This is a powerful tool for managers to analyze different scenarios, assessing the joint effect of all the involved elements.

# ACKNOWLEDGEMENTS

The authors wish to acknowledge financial support provided by CONICET (Consejo Nacional de Investigaciones Científicas y Técnicas) under Grant PIP 2706 and PIP 5914.

# REFERENCES

- Brooke, A., Kendrick D., Meeraus A., Raman, R. (1998). GAMS, A User Guide. Scientific Press, Calif.
- Corsano, G., Iribarren, O. A., Montagna, J. M., Aguirre, P.A. (2004). Batch Fermentation

Networks Model for Optimal Synthesis, Design and Operation. *Ind. Eng. Chem. Res.*, **43**, 4211 - 4219.

- Grossmann, I. E. (2002). Review of Nonlinear Mixed-Integer and Disjunctive Programming Techniques. *Optimization and Engineering*, **3**, 227 - 252.
- Paules, G. E. IV, Floudas, C. A. (1992). Stochastic programming in process synthesis: a two-stage model with MINLP recourse for multiperiod heat-integrated distillation sequences. *Computers* and Chemical Engineering, 16(3), 189–210.
- Van den Heever, S. A., Grossmann, I. E. (1999). Disjuntive multiperiod optimization methods for design and planning of chemical process systems. *Computers and Chemical Engineering*.23, 1075 – 1095.
- Vaselenak, J. A., Grossmann, I. E. and Westerberg, A. W. (1987). Optimal retrofit design in multiproduct batch plants. *Industrial Engineering Chemical Research*. 26, 718 – 726.
- Viswanathan, J., Grossmann, I. E. (1990). A Combined Penalty Function and Outer-Approximation Method for MINLP Optimization. *Comp. Chem. Engng.*, **14** (7), 769 - 782.
- Voudouris V. T.; Grossmann, I. E. (1992). Mixed-Integer Linear Programming Reformulations for Batch Process Design with Discrete Equipment Sizes. *Industrial Engineering Chemical Research.* 31, 1315 – 1325.
- Zamar, S.D., Salomone, H.E., Iribarren, O.A. (1998) Shortcut Method for Multiple Task Batch Distillations. *Ind. Eng. Chem. Res*, 37, 4801 – 4807.