Design, Synthesis and Scheduling of Multipurpose Batch Plants via an Effective Continuous-Time Formulation

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Design, synthesis and scheduling issues are considered simultaneously for multipurpose batch plants. Processing recipes are represented by the State-Task Network. The proposed model takes into account the trade-offs between capital costs, revenues and operational flexibility. Both linear and nonlinear examples are studied, resulting in MILP and MINLP problems, respectively. Comparisons with another approach are presented.

Introduction

In multipurpose batch plants, a wide variety of products can be produced via different processing recipes by sharing available pieces of equipment, raw materials and intermediates, utilities and production time resources. In order to ensure that any resource incorporated in the design can be used as efficiently as possible, detailed considerations of plant scheduling must be taken into account at the design stage.

All formulations for design and scheduling of batch processes can be classified into two groups based on the time representations. Examples of discrete time formulations are found in Grossmann and Sargent (1979); Barbosa-Póvoa and Macchietto (1994). Grossmann and Sargent (1979) solved the problem of optimal design of sequential multiproduct batch processes as a mixed integer nonlinear programming (MINLP) problem. Barbosa-Póvoa and Macchietto (1994) presented a detailed formulation of multipurpose batch plant design and retrofit based on the State-Task Network (STN) description and equally-spaced fixed event time representation proposed by Kondili et al. (1993). More recently Xia and Macchietto (1997) presented a formulation based on the variable event time scheduling model of Zhang and Sargent (1996) and used a stochastic method to solve the resulting non-convex MINLP problems.

Ierapetritou and Floudas (1998a,b) proposed a novel continuous-time mathematical model for the general short-term scheduling problem of batch, continuous and semicontinuous processes. In this paper, we extend the formulation to address the problem of integrated design, synthesis and scheduling of multipurpose batch plants.

Problem Definition

Given:

- Product recipes (i.e., the processing times for each task at the suitable units, and the amount of the materials required for the production of each product);
- Potentially available processing/storage equipment and their ranges of capacities;
- Production requirement;

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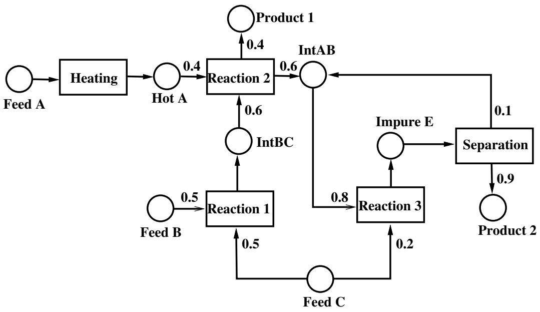

Figure 1: STN Representation

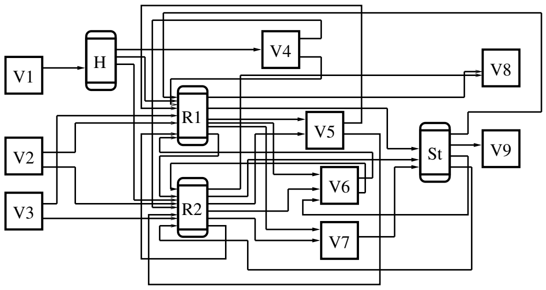

Figure 2: Plant Superstructure

- The time horizon under consideration;

Determine:

- The number, type and size of equipment items;
- A feasible operation schedule:
  - The optimal sequence of tasks taking place in each unit;
  - The amount of material being processed at each time in each unit;
  - The processing time of each task in each unit;

So as to optimize a performance criterion, for example, the minimization of the capital cost or the maximization of the overall profit.

Process Recipe and Plant Superstructure Representations

We use the concept of State-Task Network(STN) proposed by Kondili et al. (1993). Figure 1 gives an illustration of the STN description of a batch precess named KPS process. In addition to the product recipe, the information of potentially available pieces of equipment and their suitability for different tasks is used to construct a superstructure of the plant under consideration that includes all possible designs. For example, based on the KPS process recipe in Figure 1 and equipment data in Table 1, we are able to establish a superstructure of the KPS plant, as shown in Figure 2. Full connectivity of the processing units/storage vessels network is assumed.

Mathematical Formulation

To formulate the mathematical model, we require the following notation:

Indices:

i tasks; j units; s states;

n event points representing the beginning of a task;

Sets:

I tasks; I_j tasks that can be performed in unit (j); I_s tasks that either produce or consume state (s); I_p processing tasks; I_t storage tasks;

J units; J_i units that can perform task (i); J_t storage units;

N event points within the time horizon; N_l the last event point;

S all involved states; S_t states that can only be stored in storage units;

Unit	Capacity	Suitability	Task Time Model		Cost Model	
			KPSLIN	KPSNON	KPSLIN	KPSNON
Heater	20-50	Heating	1.0+0.0067b	1.0+0.0067$b^{2.00}$	100.0+0.2s	100.0+0.2s
Reactor 1	50-70	Reaction 1	2.0+0.0267b	2.0+0.0267$b^{1.25}$	150.0+0.5s	150.0+0.5$s^{1.5}$
		Reaction 2	2.0+0.0267b	2.0+0.0267$b^{1.25}$		
		Reaction 3	1.0+0.0133b	1.0+0.0133$b^{1.05}$		
Reactor 2	70	Reaction 1	2.0+0.0167b	2.0+0.0167$b^{1.15}$	120.0	120.0
		Reaction 2	2.0+0.0167b	2.0+0.0167$b^{1.15}$		
		Reaction 3	1.0+0.0083b	1.0+0.0083$b^{1.10}$		
Still	50-80	Separation	2.0+0.0033b	2.0+0.0033$b^{1.50}$	150.0+0.3s	150.0+0.3$s^{1.5}$
Vessel 4	10-30	I1(Hot A)	–	–	30.0+0.1s	30.0+0.1s
Vessel 5	10-60	I2(IntBC)	–	–	15.0+0.1s	15.0+0.1$s^{1.5}$
Vessel 6	10-70	I3(IntAB)	–	–	10.0+0.1s	10.0+0.1$s^{1.2}$
Vessel 7	50-100	I4(Impure E)	–	–	20.0+0.2s	20.0+0.2$s^{1.5}$

Table 1: Equipment Data for KPS Plant

Parameters:

r_s market requirement for state (s) at the end of time horizon;

ρ^p_{si}, ρ^c_{si} proportion of state (s) produced, consumed from task (i), respectively;

$\alpha_{ij}, \beta_{ij}, \gamma_{ij}$ constant term, coefficient and exponent of variable term of processing time of task (i) in unit (j), respectively;

H time horizon;

p_s price of state (s);

V^{min}_j, V^{max}_j minimum and maximum size of unit (j), respectively ;

$\tilde{\alpha}_j, \tilde{\beta}_j, \tilde{\gamma}_j$ constant term, coefficient and exponent of variable term of capital cost of unit (j), respectively;

Variables:

e(j) binary variables to determine if unit j exists;

s(j) size of unit j;

wv(i,n) binary variables to assign the beginning of task (i) at event point (n);

yv(j,n) binary variables to assign the utilization of unit (j) at event point (n);

b(i,j,n) amount of material undertaking task (i) in unit (j) at event point (n);

$d(s, n)$ amount of state (s) being delivered to the market at event point (n);

st(s,n) amount of state (s) at event point (n);

$t^s(i, j, n)$ starting time of task (i) in unit (j) at event point (n);

$t^f(i, j, n)$ finishing time of task (i) in unit (j) at event point (n).

Then the mathematical model involves the following constraints:

<u>Existence Constraints</u>

$$yv(j, n) \leq e(j), \ \forall j \in J, \ n \in N \tag{1}$$

<u>Unit Size Constraints</u>

$$V^{min}_j e(j) \leq s(j) \leq V^{max}_j e(j), \ \forall j \in J \tag{2}$$

Allocation Constraints

$$\sum_{i \in I_j} wv(i,n) = yv(j,n),\ \forall j \in J,\ n \in N \tag{3}$$

Capacity Constraints

$$b(i,j,n) \le V_j^{max} wv(i,n) \tag{4}$$

$$b(i,j,n) \le s(j),\ \forall i \in I,\ \ j \in J_i,\ \ n \in N \tag{5}$$

Material Balances

$$st(s,n) = st(s,n-1) - d(s,n) + \sum_{i \in I_s} \rho_{si}^p \sum_{j \in J_i} b(i,j,n-1) + \sum_{i \in I_s} \rho_{si}^c \sum_{j \in J_i} b(i,j,n), \quad \forall s \in S,\ \ n \in N \tag{6}$$

Storage Constraints

$$st(s,n) = 0,\ \forall s \in S_t,\ n \in N \tag{7}$$

Demand Constraints

$$\sum_{n \in N} d(s,n) \ge r_s,\ \ \forall s \in S \tag{8}$$

Duration Constraints: Processing task

$$t^f(i,j,n) = t^s(i,j,n) + \alpha_{ij} wv(i,n) + \beta_{ij} b(i,j,n)^{\gamma_{ij}}, \forall i \in I_p,\ \ j \in J_i,\ \ n \in N \tag{9}$$

Duration Constraints: Storage task

$$t^f(i,j,n) \ge t^s(i,j,n),\ n \in N, \tag{10}$$

$$t^f(i,j,n) = H,\ n \in N_l, \forall i \in I_t,\ \ j \in J_i \tag{11}$$

Sequence Constraints:

Same task in the same unit

$$t^s(i,j,n+1) \ge t^f(i,j,n), \forall i \in I,\ \ j \in J_i,\ \ n \in N, n \ne N \tag{12}$$

Different tasks in the same unit

$$t^s(i,j,n+1) \ge t^f(i',j,n) - H(1 - wv(i',n)), \quad \forall j \in J,\ i \in I_j, i' \in I_j,\ i \ne i',\ n \in N,\ n \ne N \tag{13}$$

Different tasks in different units

$$t^s(i,j,n+1) \ge t^f(i',j',n) - H(1 - wv(i',n)), \quad \forall i,i' \in I, j \in J_i, j' \in J_{i'}, j \ne j', n \in N, n \ne N \tag{14}$$

These constraints are written for different tasks (i, i') performed in different units (j, j') but take place consecutively according to the production recipe.

"Zero-wait" condition

$$t^s(i,j,n+1) \le t^f(i',j',n) - H(2 - wv(i,n+1) - wv(i',n)) \quad \forall i,i' \in I,\ j \in J_i, j' \in J_{i'},\ n \in N,\ n \ne N \tag{15}$$

Combined with Constraints (13) and (14), these constraints enforce that task (i) at event point (n+1) starts immediately after the end of task (i') at event point (n) if both of them are activated.

Time Horizon Constraints

$$t^f(i,j,n) \leq H, \quad \forall i \in I, j \in J_i, n \in N \tag{16}$$

$$t^s(i,j,n) \leq H, \quad \forall i \in I, j \in J_i, n \in N \tag{17}$$

Objective: Minimize

$$\sum_j (\tilde{\alpha}_j e(j) + \tilde{\beta}_j s(j)^{\tilde{\gamma}_j}) - \sum_s \sum_n p_s d(s,n) \tag{18}$$

The objective is to minimize the capital costs of units minus profits due to product sales. Other performance criteria also can be incorporated easily.

We should note that due to the nonlinear models of processing time and capital cost, the resulting mathematical programming model is a nonconvex MINLP problem, which needs deterministic global optimization methods to determine the global optimal solution.

Computational Study

The above mathematical formulation is applied to an example taken from Xia and Macchietto (1997). The process recipe, equipment data and plant superstructure are those we visited in a previous session (see Figure 1, Table 1 and Figure 2, respectively). The production requirements for Product 1 and Product 2 are 40 and 60 respectively in the linear case of KPSLIN, while 20 and 30 respectively in the nonlinear case of KPSNON. The prices of Feed A, Feed B, Feed C, Product 1 and Product 2 are 0.001, 0.002, 0.0015, 0.02 and 0.03, respectively. The time horizon under consideration is 12 hours. MINOPT, an advanced modeling language and algorithmic framework proposed by Schweiger and Floudas (1997), is used to establish and solve the resulting MILP/MINLP mathematical programming problems. The MILP problems are solved using CPLEX, a branch and bound method.

Table 2 shows the results of the proposed formulation compared with the results found in literature. Xia and Macchietto (1997) transformed the formulation they presented into an alternative one without giving the necessary details of the transformation. In addition to the reported data of the transformed formulation, the corresponding data we obtain according to their original one are also presented here. It is shown that the formulation proposed in this paper has the following advantages: (i) It gives rise to a simpler mixed-integer optimization problem mainly in terms of a smaller number of binary variables. (ii) The optimal solution obtained corresponds to a better objective function value and consequently a better integrated design and scheduling strategy. (iii) The computational efforts required are significantly reduced, which makes it very promising to solve large-scale industrial problems.

Conclusions

In this paper, a continuous-time formulation is proposed for the design, synthesis and scheduling of multipurpose batch plants. A computational study is presented to demonstrate the effectiveness of the proposed formulation. The computational results are compared with those in literature and show that the proposed formulation results in smaller size MILP/MINLP mathematical models primarily in terms of binary variables and better objective values can be accomplished with significantly less computational efforts.

Acknowledgments

Case	Formulation	Cost ($\$10^3$)	Integer Variables	Continuous Variable	Constraints	CPU (sec)
KPSLIN	Xia and Macchietto (1997)	585.62	62^t	34^t	122^t	2407.62^*
			288^o	201^o	425^o	
	This Work	572.898	128	341	877	22.49^{**}
KPSNON	Xia and Macchietto (1997)	495.11	62^t	34^t	122^t	7849.23^*
			288^o	201^o	425^o	
	This Work	490.433	108	287	722	7.31^{**}

Table 2: Results and Comparisons (t: reported based on transformed formulation; o: recounted based on original formulation; *: Sun Ultra station-1 ; **: HP-C160 workstation)

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References

Barbosa-Póvoa A. and Macchietto S., 1994, Detailed design of multipurpose batch plants. *Comp. Chem. Engng.* **18**, 1013–1042.

Grossmann I. and Sargent R., 1979, Optimal design of multipurpose chemical plants. *Ind. Eng. Chem. Process Des. Dev.* **18**, 343–348.

Ierapetritou M. and Floudas C., 1998a, Effective continuous-time formulation for short-term scheduling: I.multipurpose batch processes. *Ind. Eng. Chem. Res.* **37**, 4341–4359.

Ierapetritou M. and Floudas C., 1998b, Effective continuous-time formulation for short-term scheduling: Ii. continuous and semi-continuous processes. *Ind. Eng. Chem. Res.* **37**, 4360–4374.

Kondili E., Pantelides C., and Sargent R., 1993, A general algorithm for short-term scheduling of batch operations -i. milp formulation. *Comp. Chem. Engng.* **17**, 211–227.

Schweiger C. and Floudas C., 1997, *MINOPT : A Software Package for Mixed–Integer Nonlinear Optimization, User's Guide*. Computer–Aided Systems Laboratory, Dept. of Chemical Engineering, Princeton University, NJ.

Xia Q. and Macchietto S., 1997, Design and synthesis of batch plants - minlp solution based on a stochastic method. *Comp. Chem. Engng.* **21**, S697–S702.

Zhang X. and Sargent R., 1996, The optimal operation of mixed production facilities - general formulation and some solution approaches for the solution. *Comp. Chem. Engng.* **20**, 897–904.