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# Dynamic Operations in the Planning and Scheduling of Multi-Products Batch Plants

**Tarun Bhatia and Lorenz T. Biegler**

**EDRC 06-209-95**

# DYNAMIC OPERATIONS IN THE PLANNING AND SCHEDULING OF MULTI-PRODUCT BATCH PLANTS

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**Abstract**

**Execution of tasks in dynamic batch units provides additional operating freedom via transient control profiles. When considered at the design and scheduling stage, this freedom can stretch the limits of profitability under strict market, facility and time constraints. The work in this paper-incorporatestdynamic processing conditions for products in a multi-product batch plant, as opposed to fixing the process by recipes, in the broader context of equipment design, production planning, scheduling and inventory considerations. The objective is a general function of fixed design costs, operating costs, production revenues etc. Decisions include stage processing times for products, transient stage operating policies, continuous design parameters, production capacity and production schedules. The infinite dimensional optimal control problem for each operation is solved using collocation over finite time elements ([6], [7]). Scheduling, with its combinatorial complexity, is addressed in the scope of *flowshop* plants for specific transfer policies using the *Aggregated* Scheduling model in [3] and [4]. Two examples are solved via sequential and simultaneous solution approaches. The smaller first example allows transient control at the reaction stage for problems with relevant objectives in planning and scheduling. The second example allows transient control at the reaction and high purity separation stage for a general objective function. Considerable savings achieved in most situations are reported, along with moderate computational requirements for solving the examples.**

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# 1 Introduction

Specialty chemical production faces strict and varying market constraints of product quality and time. These are better addressed through flexible processing in batch plants, whose features include adjustable unit-task assignments, production schedules, storage and transfer policies etc. While much effort is directed in integrating the flexibility at different levels of a batch operation *(e.g.* [10], [4]), processing considerations are often avoided due to expensive computational and modeling requirements. In particular, batch processing decisions pertain to optimal state and control variable profiles for dynamic stages providing transient operating freedom.

At the lowest level, stage processing times and operating conditions are fixed by process recipes. While this simplifies an integrated solution for other aspects of the problem, it overlooks the potential of optimizing the dynamics at each processing stage in improving the integration. Rigorous dynamic modeling on the other hand promises improved performance at the cost of a complicated integration.

Operating considerations have been incorporated at other levels such as process development ([1]) and plant design ([9],[8]) through sequential, nested or bi-level solution approaches. Although these methods solve smaller subproblems, their solutions are often suboptimal. A general MINLP formulation for short term planning, where processing times form a sequence dictated by operating conditionsJs proposed in [11]. Mom'SEcendy^et^ed 4ynamic task models have been used in place of process recipes for a profitable operation ([5]).

The work here includes dynamic models of processing tasks within the design and scheduling formulation for a special class of batch operations. Stage operations with optimal control profiles are compared to those with best constant control levels to improve overall profit objectives. Variables treated simultaneously as decisions in this work include:

- *Processing*
  - Optimal stage operations
  - State and control variable profiles
  - Stage processing times
  - Final batch state at each production stage
- *Design*
  - Continuous equipment sizes
  - Continuous design parameters
- *Production Planning*
  - Production capacity

- Batch sizes and number of batches

- *Scheduling*

  - Production span or cycle time ,
  - Production sequence

The above problem is complicated most by solutions for optimal transient operating conditions in various processing stages. Such decisions fall under the class of infinite dimensional optimal control problems. These problems are defined by a differential-algebraic (DAE) system of equations. While the method of Control Vector Iteration used in [5] solves for control profiles, it does not handle state path constraints directly. Path constraints are essential for quality constrained batch processes. Collocation with finite elements, on the other hand, allows convenient handling of path constraints for moderately sized problems.

The other aspect that poses a problem is the combinatorial nature of scheduling decisions. To simplify the scheduling issue, this work confines itself to a special class of batch problems, i.e. flowshop plants with Unlimited Intermediate Storage (UIS) and Zero Wait (ZW) transfer policies and with one unit per stage.

# 2 Problem Formulation and Modeling

This section discusses measures taken to counter the complicating issues in the overall problem as presented in section 1. Formulations for modeling different aspects of the problem are also presented.

## 2.1 Processing and Design

Modelling dynamic processes in batch stages requires differential and algebraic equations involving state and control variables. The optimization problem can be written as:

$$
\begin{aligned}
\bullet \quad & \max \quad \#r(t)_f u(0,*(*/)_f p) \\
\text{s.t.} \quad & i(«) = /(*(«), u(t), p) \\
& g(z(t)Mt), p) \leq 0 \\
& g_e(z(t_e), u(t_e), p) \leq 0 \\
& h(z(t), u(t), p) = 0 \\
& h_e(z(t_e), u(t_e), p) = 0 \qquad \text{(DAE)}
\end{aligned}
$$

where *t/j* is the objective function,
*z(t)* is the vector of state trajectories,

| | |
|---|---|
| $u(t)$ | is the control profile, |
| $p$ | are continuous parameters, |
| $tf$ | is the stage processing time, |
| $\leq j, h$ | are inequality and equality path constraints, |
| $g_e, h_e$ | are end point constraints at the initial and final time, |
| $t_t$ | are initial and final time. |

The method of Orthogonal Collocation over finite elements transforms this infinite dimensional problem to a finite dimensional NLP problem. In this method, time is divided into a number of elements and the state and control profiles in each element are approximated by Lagrange polynomials of appropriate order, equations ( 1 and 2). Coefficients for these polynomials are then treated as decisions in the exact solution for the system at collocation points within each time element.

$$z_l(\tau) = \sum_{m=0}^{ncol} z_{lm}\phi_m(\tau) \quad \forall l; \quad \phi(r) = \prod_{m'=0;m'\neq m}^{ncol} \frac{\tau - \tau_{m'}}{\tau_m - \tau_{m'}} \tag{1}$$

$$u(r) = \sum_{m=1}^{ncol} u_{lm}\theta_m(r) \quad \forall l; \quad \theta_m(r) = \prod_{m'=1,m'\neq m}^{ncol} \frac{\tau - \tau_{m'}}{\tau_m - \tau_{m'}} \tag{2}$$

| | |
|---|---|
| where $l$ | are finite time elements (l,...,ne), |
| m | are collocation points (l,...,ncof), |
| r | is normalized time in each element, r € {0,1] |
| $r_m$ | are normalized roots of Legendre polynomials |
| z/m, w/m | are state and control profile parameters, |
| $\theta_m(t)$ | are basis functions for Lagrange polynomials, |

Division of the profile into elements allows control variable discontinuities to exist, as in bang-bang control. Continuity of the state profile is enforced across neighboring elements, for this purpose the order of the state approximation is kept one higher than the control. The order of approximations and location of collocation points are determined by stability and error properties of the system. The model is exactly satisfied at collocation points and the approximation error is controlled within each element. Using this technique the resulting NLP problem then is of the form :

$$\max_{z_{lm},u_{lm},p,t_f} \psi(z_{lm}, u_{lm}, t_f, p)$$

$$\text{s.t.} \quad z(T_m) - S_{rif}(z_{Lm}, u_{lm}, p) = 0$$

$$g(z_{lm}, u_{lm}, p) \leq 0 \quad \forall l, m$$

$$g_e(z_{lm}, u_{lm}, p, t_e) \leq 0 \quad \forall l, m$$

$$h(z_{lm}, u_{lm}, p) = 0 \quad \text{V/,m}$$
$$h_e(z_{lm}, u_{lm}, \text{P,te}) = 0 \quad \text{V/,m}$$
$$z_{l+1,0} = \sum_{\text{m'}=0}^{ncol} z_{lm}\phi_m(1) \quad \forall l; \quad l \neq ne$$
$$\sum_l \delta\tau_l = t_f \qquad \text{(NLPl)}$$

where <$IJ is the length of finite time element /,

$ti_m$ is the absolute time at point m in element /.

note $Um = Y!P\sim1\backslash **l' + \delta\tau_l\tau_m$

Properties of this method in solving for optimal control profiles together with design decisions, are discussed in [6] and [7].

## 2.2 Production Planning and Scheduling

Performance of periodic schedules can be characterized approximately by a cycle time. To allow gradient based optimization, a closed form expression for the cycle time must exist. The expression must model the combinatorial complexity of the scheduling problems. This is challenging due to the sequence in which processing stages are required for making a product as well as the sequence in which product batches are made. An increase in either the number of products or their batches adds to this complexity. Simplifying assumptions or special cases must therefore be considered. Within the realm of flowshop problems, the Unlimited Intermediate Storage (UIS) and Zero Wait (ZW) policies permit sequence dependence to be contained in a closed form expression, as shown in [3].

In flowshop problems, all products require processing stages in the same sequence. Production sequence is then handled relatively simply when considering two special transfer policies.

UIS assumes an infinite storage facility at zero cost. This implies that a stage, after processing a batch, becomes immediately available for processing the next one. This is possible as the current batch can be moved to storage in the event the next stage is still busy. Infinite storage thus has the effect of decoupling successive stages. The cycle time for a stage then simply becomes the total time required for processing all batches in that particular stage and sequence dependence is eliminated from the problem.

ZW requires a batch be transferred to the next stage immediately after its completion in the current one. This rigidity ensures availability of the current stage to process the next batch as soon as the previous one is done, like in UIS. In addition, a batch must be started at the first stage only when it can be processed through each stage without delay. This leads to slacks or idle times to exist at all stages but one (at least), the bottleneck stage, whose location

depends on the previous product in the sequence. Cycle time for a stage with ZW policy thus becomes sequence dependent due to the slack times, the problem is however tractable in the "aggregated" space of product pairs.

These ideas are exploited in [3], where the "aggregated" model (Ml) is proposed to perform simultaneous production planning and vessel sizing for a least design cost flowshop plant. It handles ZW and UIS policies, assuming one unit per processing stage but considers recipe based processes with fixed processing times for products in all stages.

$$\min \sum_{j=1}^{J} \alpha_j V_j^{\beta_j}$$

$$\text{s.t.} \quad Vj \geq S\hat{}Bi \quad \forall i,j \tag{3}$$

$$m = \frac{\%}{D_i} \quad \forall i \tag{4}$$

$$\sum^{N_p} NPRS_{ik} = m \quad \forall i \tag{5}$$

$$\sum^{N_p} NPRS_{ik} = n_k \quad \forall k \tag{6}$$

$$\sum_{i=1}^{N_p} \left( \text{I}''** + \sum_{k=1}^{N_p} SlikjNPRS* \text{J} \right) \leq \text{H} \quad \forall i \tag{7}$$

$$SL_{ik,j} + t_{k,j} = t_{i,j+1} + SL_{ik,j+1} \quad \forall t\backslash j,*; \quad j \hat{} J \tag{8}$$

$$NPRS_{ii} \leq n_i - 1 \quad \forall t \tag{9}$$

$$Vj\hat{}O.ni\hat{}O.BitO.NPRSik\hat{}O \qquad \text{(Ml)}$$

where $j$ are stages in flowshop sequence (1,..,J),
t,fc are products (l,...,iVp),
a j, /Jj- are design cost co-efficients,
$Vj$ are continuous equipment size parameters,
$Sij$ are size factors for product $i$ in stage j,
Bt is the size of all batches of product i,
fit is the number of batches of product i,
$Qi$ is the amount of product $i$ produced,
$NPRSik$ is the number of product sequence $ik$ pairs in the schedule,
$Uj$ is the processing time for product t at stage j,
$SLikj$ is the ZW slack at stage $j$ for product sequence pair $ik$,
$H$ is the planning horizon.

The objective is to minimize fixed equipment costs although a more general objective could be accommodated within the formulation. The equipment is

designed large enough to accommodate all batches through equation( 3). Sufficient batches of each product that satisfy market demands are ensured by equation( 4). Equations ( 5) and ( 6) require a product to appear an appropriate number of times in each product pair. Equation ( 9) eliminates single product subcycles from appearing in the schedule. Equation ( 7) ensures the chosen schedule is completed in the available horizon.

The left hand side expression in equation( 7) models the cycle time at a stage. In the context of ZW policy, a stage *j* becomes a bottleneck for a product sequence pair *ik* if there is no idle time at this stage, i.e. *SLikj* is zero. For the sequence independent UIS policy, all slacks must be set to zero. The number of product pairs in the solution generate a family of schedules each having the same cycle time. As discussed in [3], the makespan, or total time for which the plant must be run depends on which product pair is split in the schedule family.

Figure 1: *Calculation of slacks with "free" processing times.*

When processing times *Uj* are fixed, an off-line slack calculation for each pair would suffice. Considering dynamic processing freedom in this framework must allow processing times *Uj* to vary and adopt optimal values that reduce the overall idle times in the optimal schedule family. This would require variable slacks *SLikj* causing the bottleneck stage location for each product pair to shift during the solution. Discontinuities in the presence of such effects can be avoided by ensuring feasible slack calculation via equations( 8), which must be included as developed in [2]. Allowing variable processing and slack times in the formulation introduces bi-linear terms in the expression for cycle time.

The reliance on size factors to determine equipment sizes is inadequate when considering process dynamics. For instance, different operating strategies can cause different size batches to be realized in the same equipment. Since the overall problem allows general operating profiles that are solved together with continuous design parameters, feasibility of design is maintained for the multi-product operation more rigorously. Size factors could still be used in forming a resource function for stages that do not involve any modeling.

## 2.3 Overall Formulation

Problem formulation for simultaneous solution of all decisions in this work is based on the representation in Figure 2. A total of *J* processing stages, in the flowshop sequence, are considered for the production of $N_p$ product batches of size *Bi* for each product *i*. Variables *z®j* and *z{;* denote the initial and final state of a batch of product *i* at stage *j*. The state trajectories *Zij(t)*, for which these variables are the boundary values, depend on the control profile *U{j(t)*

implemented for product *i* at stage *j*. Units that are modeled dynamically belong to a subset *K*. All units allow continuous design parameters *pj* to be treated as decisions. Before the detailed problem formulation is presented, an informal organization of interactions in the overall problem is presented.

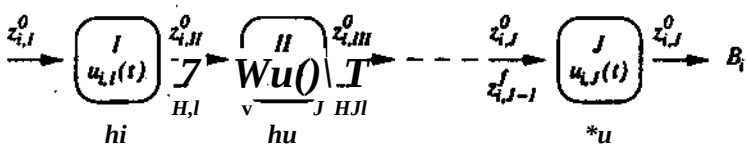


Figure 2: *Problem representation.*

Starting with stage operations for units that are modeled dynamically, different levels of process modeling can be considered that relate processing time with equipment design and batch states. At the highest level lie dynamic models (DAE) that allow a general control profile within specified operating bounds. At lower levels, the operating profile structure can be specified such as piece-wise constant, piece-wise linear or best constant operating level. This can be achieved by placing constraints on the coefficients in the approximation for the control profile. Processing time in these units depend on system dynamics, design parameters and initial and final states. Units not modeled dynamically could still have processing time as a function of material transformation achieved in the unit, possibly allowing some operating parameter decisions. Finally, recipe based tasks, that provide no freedom as far as processing time or material transformations are concerned, lie at the lowest level. All descriptions for residence time of a batch in a unit are a special case of equation 10.

$$t_{ij} = \phi_t(z_{ij}(t), u_{ij}(t), z^0_{ij}, z^f_{ij}, p_j) \quad \forall i, j \tag{10}$$

Movement of a batch in the flowshop sequence requires starting conditions at each stage to be determined by final conditions at the previous unit in the sequence. For the case where material is added only at the first stage and recovered only at the last one with unaltered batch transfer at intermediate stages, initial conditions would be given by equation 11.

$$* \& = * \& - ! \quad \forall t, i; \quad j * l \tag{11}$$

When the initial and final state of all product batches at each processing stage are fixed by recipes, dynamic optimization of the process at each stage would realize specified transformations more efficiently. In this situation, stage operations are decoupled as far as material state transformations are concerned. Operation in a stage is however affected by processing time requirements at other stages. In the more general context, when batch state trajectories as well as their intial and final conditions at all stages are treated as decisions, control

over a product batch size is determined more strongly by the operations and design of all stages through equation 11.

$$B_i = 4>B(Uj,Uij(t),z_{ij}(t),p_j) \quad \text{Vt} \tag{12}$$

Size of a product batch dictates the number of batches, which along with processing times determine the optimal schedule cycle time at each stage.

$$CTj = 4>CT\{t_{ih}ni(Bi),\ NPRS_{ik}) \quad \text{Vj} \tag{13}$$

Ideally n« and *NPRSik* must be integers. Although this is guaranteed under special conditions ([2]), for recipe processes, these and other integer design variables could be treated as continuous to get a relaxed solution that is refined further. The overall NLP model for the problem then becomes:

$$\max_{z_{ijlm},u_{ijlm},p_j,\delta\tau_{ijl}} \quad \psi_{profit}(CT_j, V_j, Q_i)$$

s.t.

$$z'ij(ri_m) - <STijlf(Zi_{jlm}\ ,u_{ijlm},p) == 0 \quad Vi,j,l,m$$

$$9(Zijlm,Uij\ lm,P) \leq 0 \quad \text{Vi,j},l,m$$

$$9e(Ziji,Uiji\ ,tiJ,p) \leq 0 \quad \text{Vi,j}; \quad / = \text{ne}$$

$$h(ziji_m,Uij\ lm,p) = 0 \quad \text{Vi,jf,Z,m}$$

$$he(Zijt,Uiji\ ,Uj,p) = O \quad \text{Vi.i;}\ / = \text{ne}$$

$$z^L_{ijlm} \leq z_{ijlm} \leq z^U_{im}$$

$$U^L_{ijlm} \wedge z_{ijlm} \leq z^U_{ijlm}$$

$$t_{ij} = \sum_l \delta\tau_{ijl} \quad \forall i,j$$

$$z^0_{ij} = z_{ij10} \quad \text{Vt,i}$$

$$*M+W - \sum_{m'=0}^{ncol} z_{ijlm}\phi_m(1) \quad \forall i,j,l; \quad l \neq ne$$

$$z^f_{ij} = \sum_{m'=0}^{ncol} z_{ijilm}(1) \quad \text{1Vt,j,Z;} \quad \text{Z} = \text{ne}$$

$$z^0_{ij} = f(z^f_{i,j-1}) \quad \forall i,j; j \neq 1$$

$$B_i = f(z^f_{ij}) \quad \forall i,j = J$$

$$V_j \geq S_{ij}B_i \quad \forall i,j$$

$$n_i$$

$$\sum_{*=1}^{N_p} NPRS_{ik} \wedge rii \quad \text{Vf}$$

$$\sum_{i=1}^{N_p} NPRS_{ik} = n_k \quad \forall k$$

$$NPRS_{ik} \le n_k \quad \forall i$$

$$CT_j = \sum_{i=1}^{N_p} \left( n_i * t_{ij} + \sum_{k=1}^{N_p} SL_{ikj} NPRS_{ik} \right) \quad \forall j$$

$$CT_j \le H \quad \forall j$$

$$SL_{ikj} + t_{ij} = t_{ij+1} + SL_{ik+1j} \quad \forall i, k, j \quad j < J$$

$$\forall j \ge 0,\ n_i \ge 0,\ NPRS_{ik} \ge 0,\ t_{ij} \ge 0,\ SL_{ikj} \ge 0 \qquad \text{M2}$$

where $Z_{ijm}$ are state coefficients for product $i$ in stage $j$,
$U_{ijm}$ are control coefficients for product $i$ in stage $j$,
$S_{rij}$ is the Z element length for operation $ij$,
$profit$ is the objective function,
$Z_{ij}(t)$ is the state expression in element / for operation $ij$,
$U_{ij}(t)$ is the control expression in element / for operation $ij$,
L, $U$ represent lower and upper bounds,

# 3 Examples

The overall formulation is **used** to **demonstrate improved** objective function **values when** considering process dynamics **for relevant situations in planning** and scheduling. Two flowshop examples are **constructed for this** purpose. The first example is kept small for **motivating purposes. A larger problem** is solved next, sequentially as well as simultaneously, to understand **some** of **the** tradeoffs more closely.

## 3.1 Example 1

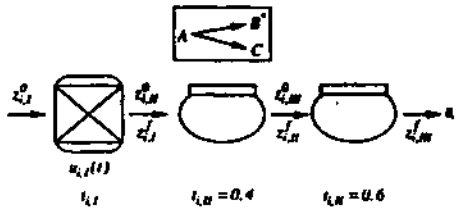


Figure 3: *Example 1 (dynamic reactor).*

Three products, very similar in process, are to be made in a flowshop plant (Appendix A). All products require three stages, a dynamic reactor and two recipe based blenders (figure 3). The reaction mechanisms for all products are similar as products differ only in the kinetic parameter values.

A control profile *Uij(t)* exists for each product *i* in the reactor. Initial feed charge in the reactor is fixed for each run. Dynamic control is then expected to improve conversion of this charge to the desired product both in time and extent, with competing reactions. Four problems involving scheduling, design and processing tradeoffs are solved with constant and transient reactor control profiles, for both the UIS and ZW policies.

- **PI - Minimize Operating Cost**

  Minimize operating costs to achieve a production target in an existing facility.

- **P2 - Minimize Fixed Costs**

  Minimize equipment costs to achieve a production target in a specified horizon.

- **P3 - Maximize Revenues**

  Maximize revenues from operating in an existing facility for a specified horizon.

- **P4 - Maximize Overall Profit**

  Maximize an overall profit function of fixed costs, operating costs and net revenues.

### 3.1.1 Solution Strategy

Control profile ttt,/(t) is resolved using four equal sized finite elements spanning the processing time for each operation. Two collocation points are introduced within each element. Intensive composition trajectories serve to define the dynamic system state. Equipment sizes are then related to product batch sizes through size factors.

Problems PI - P4 are solved successively, for both UIS and ZW policies, such that solution for one problem provides an initialization to the next one. Problems PI are initialized by solving individual reactor subproblems that maximize conversion to each product in 1 hour. For problems PI, equipment sizes and production targets are fixed. In problems P2, equipment sizes are relaxed and stage cycle times are bounded by a horizon constraint. For problems P3, equipment sizes are again fixed and production targets bounded from below. Finally, for problems P4, equipment sizes and stage cycle times are relaxed and production is bounded from above.

### 3.1.2 Results

For all problems, performance with the idealized UIS policy is better than with the more constrained ZW policy (figure 4). In addition, dynamic control profiles improve most cases beyond operating at the best constant level.

Reactor control profiles for a typical case are shown in figure 5. Operating at the best constant control level starts off with a high conversion rate that reduces

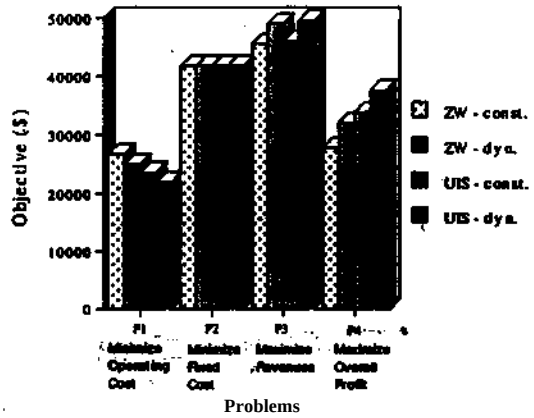


Figure 4: *Results for example 1.*

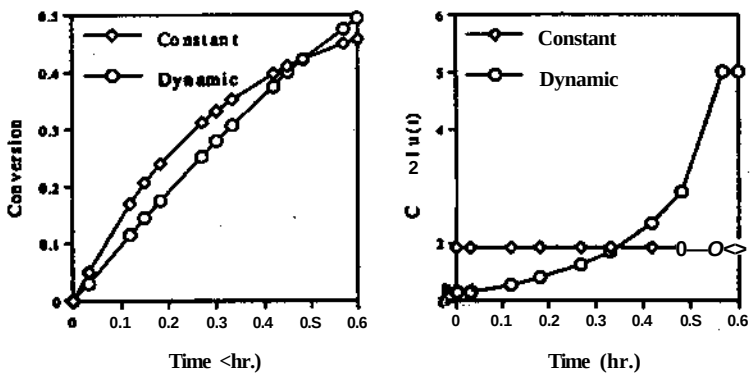


Figure 5: *Optimal profiles (product 1, problem P2, ZW policy).*

as the reaction proceeds. An optimal profile roughly maintains the same steady conversion rate throughout the operation. The difference in strategies becomes significant close to the end of the operation, giving larger batches for the optimal operation.

**Problem PI - Minimize Operating Cost**

With ZW policy, operating costs reduce by 6.8% for the dynamic case (table 1). The reactor processes each product for 0.6 hours with both constant and transient control. This eliminates slack times from two stages out of the three, for all product pair combinations. A higher conversion with dynamic control produces larger sized batches for all products. As a result fewer batches suffice to meet production targets. Stage cycle times are thus reduced with dynamics

| Problem PI | ZW | |
|---|---|---|
| | const. 0=26,72$ | dyn. 0=24,922 |
| $CT_i$ (hr.) | 190.9, 190.9, 190.9 | 178.0, 178.0, 178.0 |
| $x_i$ | 0.459, 0.492, 0.414 | 0.495, 0.527, 0.442 |
| $U_j$ (hr.) | 0.6, 0.6, 0.6 | 0.6, 0.6, 0.6 |
| **Problem PI** | **UIS** | |
| | const. 0=23,5^8 | dyn. 0=22,025 |
| $CT_i$ (hr.) | 153.9,143.0, 214.5 | 145.7, 132.8, 199.2 |
| $x_i$ | 0.387, 0.411, 0.412 | 0.422, 0.445, 0.435 |
| $U_j$ (hr.) | 0.360, 0.343, 0.594 | 0.377, 0.359, 0.581 |

**Table 1:** ***Results for problem PL***

even though reactor processing times in both cases are the same.

With UIS policy, 6.4% is saved by considering dynamics in the reactor. Unequal cycle time values for each stage are a result of decoupling between successive stages for the UIS case. Processing times are lower than 0.6 hours as any improvement in time benefits the cycle time with UIS. Batch sizes are thus smaller than in ZW case, due to shorter processing in the reactor. Dynamic control still produces larger batches although, with slightly longer reactor operations. The reduction in number of product batches that satisfy demands however compensates this increase in processing times. Cycle time is thus reduced in all stages for the dynamic case, although the reduction is not as significant as in the ZW case.

**Problem P2 - Minimize Fixed Costs**

| Problem P2 | ZW | |
|---|---|---|
| | const. 0=41,785 | dyn. 0=41,641 |
| $V_j$ (1.) | 107.0, 111.5, 113.0 | 106.6, 111.2, 112.5 |
| $x_R$ | 0.459, 0.446, 0.395 | 0.463, 0.444, 0.395 |
| $U_j$ (hr.) | 0.6, 0.440, 0.549 | 0.499, 0.385, 0.478 |
| **Problem P2** | **UIS** | |
| | const. 0=41,641 | dyn. 0=41,641 |
| $V_j$ (1.) | 106.6, 111.2, 112.5 | 106.6, 111.2, 112.5 |
| $x_R$ | 0.463,0.444,0.395 | 0.463, 0.444, 0.395 |
| $U_j$ (hr.) | 0.650, 0.451, 0.543 | 0.510, 0.357, 0.477 |

**Table 2:** ***Results for problem P2.***

Fixed costs reduce by a mere 0.34% for ZW policy with a dynamic profile (table 2). This slight reduction is achieved by permitting the reactor to process batches of slightly smaller size for product 2, which requires larger equipment than others. Reaction is stopped for other products when their batches exceed

the limit placed by equipment sizes corresponding to product 2. This permits slack times to exist in the reactor for almost all product pairs with both constant and dynamic control.

UIS shows no improvement for problem P2 with dynamics. Conversion to products, and hence batch sizes, are the same as in the ZW case with dynamics for both constant and dynamic UIS cases. The two UIS solutions differ in reactor processing times for products. Both cases still allow longer processing in the reactor than corresponding ZW cases. This is possible since the horizon constraint is not active at these solutions. Results for problem P2 reflect small sensitivity of fixed costs to introducing dynamics in the reactor.

**Problem P3 - Maximize Revenues**

| Problem P3 | ZW | |
|---|---|---|
| | const. V>=45,433 | dyn. t/>=48,995 |
| *mBi* (lb.) | 4800, 5545, 4800 | 4800, 6732, 4800 |
| $x^J_R$ | 0.459, 0.492, 0.414 | 0.495, 0.527, 0.442 |
| *Uj* (hr.) | 0.6, 0.6, 0.6 | 0.6, 0.6, 0.6 |
| Problem P3 | UIS | |
| | const. ^=45.866 | dyn. ^=49,357 |
| *TiiBi* (lb.) | 4800, 5688, 4800 | 4800, 6852, 4800 |
| *'« | 0.438, 0.463, 0.476 | 0.476, 0.501, 0.501 |
| *Uj* (hr.) | 0.519,0.493,0.818 | 0.535, 0.510, 0.797 |

**Table 3:** ***Results for problem P3.***

An improvement of 7.8% is observed with dynamics for ZW policy (table 3). At the solution minimum demands are satisfied for all products. Beyond these, production of product 2 is increased as revenues from its sales are the largest. Conversion and processing time decisions are same as for corresponding PI problems. The specified horizon is larger than stage cycle time values in PI. Extra batches of product 2 are processed until the horizon constraint becomes active. Dynamics allow a greater number of larger batches of product 2 to be accommodated in the available horizon.

With UIS, increased production with dynamics improves the objective by 7.6%. Higher conversions are achieved with slightly longer*processing times in the reactor, although product 3 behaves otherwise. While both policies operate under the same horizon constraint, production is higher with UIS due to zero slacks at the stages.

**Problem P4 - Maximize Overall Profit**

Overall profit is increased a little over 15% when reactor dynamics are considered with the ZW policy (table 4). Production reaches the upper bound for all products in both cases. A higher conversion is achieved for all products in the dynamic reactor. As a result, fewer batches exist in the schedule leading

| Problem P4 | ZW | |
|---|---|---|
| | const. t/>=27,641 | dyn. t/>=31,848 |
| CT; (hr.) | 397.7, 397.7, 397.7 | 370.9, 370.9, 370.9 |
| $V_j$ (L) | 118.0, 123.0, 120.5 | 126.6, 131.8, 129.2 |
| $x_B^j$ | 0.459, 0.492, **0.414** | 0.495, 0.527, **0.442** |
| $U_j$ (hr.) | 0.6, 0.6, **0.6** | 0.6, 0.6, 0.6 |
| **Problem P4** | UIS | |
| | **const. V=33,707** | **dyn. V=37,371** |
| CTi (hr.) | **354.6, 279.7, 419.6** | **334.9, 259.9, 389.8** |
| $Y_s$ 0 0 | **119.3, 123.7, 125.9** | **125.9, 130.6, 132.9** |
| $x_B^p$ | **0.411, 0.435, 0.442** | **0.448, 0.472, 0.466** |
| tt./(hr.) | **0.429, 0.408, 0.691** | **0.447, 0.426, 0.676** |

Table 4: *Results for problem P4.*

to smaller cycle times for the dynamic case, at the cost of a slight increase in equipment sizes to accommodate the bigger batches.

With UIS policy, the increase in overall profit is 10.9% due to smaller variations in cycle time or equipment sizes. With optimal reactor control, higher conversions are achieved in larger processing times for each product. This gives a schedule with **fewer larger** isized batches that performs better over the case with a best operating level.

It is interesting to note that deriving the exact product sequence for all problems studied is simple. UIS problems are sequence independent as discussed earlier in this work. For ZW problems, with the exception of problem P2, all products require processing in the reactor for the same time. Also, the reactor becomes a bottleneck stage in all problems. **All** products thus become identical in processing time requirments and this special condition renders the ZW case to be sequence independent too. Determination of the exact makespan from the family of schedules is similarly simplified. However, number of product pairs at the solution for most cases reflect single product campaigns.

| **Problem** | **ZW** | | **UIS** | |
|---|---|---|---|---|
| | | **dyn.** | **const.** | **dyn.** |
| PI | 0.390 | **0.370** | **0.310** | **0.300** |
| **P2** | **0.390** | **0.360** | **0.310** | **0.300** |
| **P3** | **0.360** | **0.310** | **0.350** | **0.310** |
| **P4** | **0.410** | **0.390** | **0.380** | **0.310** |

Table 5: *CPU seconds for solving example 1 using the NLP solver CONOPT through the GAMS modeling system on an HP 9000/700 workstation.*

This motivating example reflects some of the benefits in including dynamic process models for different aspects of batch operations. A simultaneous integration of process considerations is achievable with modest computational

requirements under the assumptions inherent in this work.

## 3.2 Example 2

A flowshop plant with four units, a reactor, a heat exchanger, a separator and a binary distillation column converts feed of a fixed quality to three products of different purity in the desired component (P). A total of three reactions occur in the reactor, involving six components. Product P formed in the second reaction, reacts to a waste G that separates when the mixture is sufficiently cooled in the heat exchanger. All of waste G is then removed in the separator and the remaining five component mixture is fed to the distillation column. Heat exchanger and separator operations are modeled along recipes, with processing times for all three products in these two units being fixed. No processing freedom exists in these two operations.

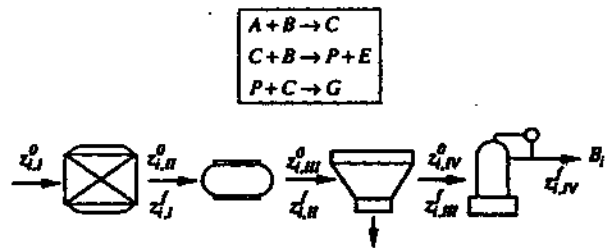


Figure 6: *Example 2, (dynamic reactor and distillation column).*

Separation of the waste free material into high (P) purity products is achieved in the distillation column. The column treats the feed for each multi-period run as a binary one, where the first component is the desired product (P) and the second a pseudo-specie of other intermediate and feed components remaining in the mixture. Feed quality at the start of a column run is arrived at by a waste G-free calculation on the final state of the reactor charge. This corresponds to the separation unit, and consumes no degrees of freedom.

### 3.2.1 Solution Strategy

For reactor dynamics (problem details given in Appendix B), the alloted processing time is discretized using eight finite time elements with 2 collocation points each. To capture the steep initial part of the profile, four smaller sized elements are used at the start and four larger elements are used for the rest of the profile. Intensive weight fractions for five components out of the six present represent the state at any time. This allows an optimal temperature profile to remain valid for a scale up in the extensive initial charge in the reactor. Reactor operations for each product are identical in processing time, final state and temperature profiles for all products. Product batches gain identity only in the distillation column.

Column dynamics axe solved using the short-cut batch distillation model in [7] without hold-up. Four finite equal sized time elements with 3 collocation points span the processing time to determine the optimal reflux profile for each operation. For a binary feed, the model involves one intensive composition (xci(O) ^d $^{one}$ extensive load (5(0) variable. Apart from the residual equations, other equations satisfied at the collocation points include equilibrium relations, Gilliland's correlation and Underwood's equations. Appropriate purity constraints specify the product that is to be produced during any period. Multi-period runs that produce the same product are also identical as in example 1, implying that processing time, batch size and reflux profile for a product in the column would be identical for all batches of that product irrespective of their position in the schedule.

The reactor thus produces as much of P and the column separates it according to specifications. Cooling and waste separation both require a time of 0.5 hours for all products.

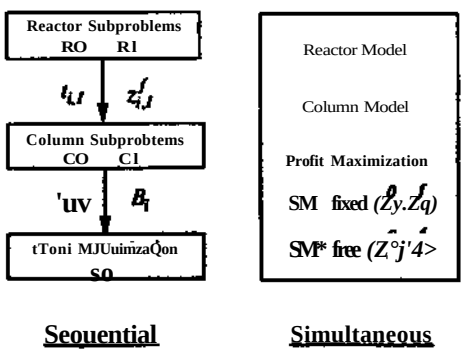


Figure 7: *Solution strategies adopted for example 2.*

An overall profit objective is maximized sequentially as well as simultaneously for the ZW policy. For the sequential case, unit subproblems are first solved to generate processing time and batch size data that is used in maximizing profit. In the simultaneous approach, dynamic models for the units are included in profit maximization treating processing times and batch sizes as decisions only. The final condition of the batches at the reactor, and thereby the initial condition of the batches at the column, are constrained at values determined by the sequential approach. In the last case, final condition at the reactor and initial condition for the column are also included as decisions. Problems are solved for combinations of reactor/distillation column operating modes. This strategy is discussed in detail next.

### 3.2.2 Problem Formulation

#### Unit Subproblems

For sequential solution, unit subproblems R0-C1 are solved first for the optimal temperature and reflux profiles in the reactor and column respectively, with

different perceived objectives. For column operations, a constant initial charge and number of trays are used for all problems.

Reactor subproblems first maximize conversion to desired product in an allocated time of one hour with the best constant operating temperature (Case RO). A general transient profile is then allowed (Case Rl) and the problem resolved for the shortest time that gives the same final state as in RO. The column problems are similarly solved, first with the best constant reflux levels to separate the largest product batches in an allocated time of two hours (Case CO) and then allowing an optimal reflux profile to separate an equal batch in the shortest time (Case Cl).

$$zf = \max^{\wedge} / (* '_{i}) \quad st.(t_{iff} = l) \quad Vi \qquad \text{(RO)}$$

$$min_{Tilit)} \; Uj \; sX.(z\{j = zf \; °) \; Vi \qquad \text{(Rl)}$$

$$Bf° = m*Xn_{iJV}Bi \quad s.t.\{Ujv = 2, \quad z?_{f/l}, = /(*\{/)) \quad Vi \qquad \text{(CO)}$$

$$****.,vm*ijv \quad {}^{st} - « / v = /(*£/). \quad B|>£lf°) \quad Vi \qquad \text{(Cl)}$$

where $zf°$ is the final state in reactor for problem RO,
$\overline{T}u$ is the best constant temperature for product i,
$Tu(t)$ is the optimal temperature profile for product i,
$Bf^{Q}$ is product i batch size for problem CO ,
$\overline{R}ijv$ is the best constant reflux for product i,
$Rijv(t)$ is the optimal reflux profile for product $i$ ,
$z®_{IV}$ is the initial condition for a batch in the column,
$z\{j$ is the final condition of a batch in the reactor.

Processing time and batch size data from solving these subproblems are used in maximizing profit for four different operating combinations, depending on whether the data chosen for a dynamic unit corresponds to an optimal profile or a constant operating level. This corresponds to the sequential (SQ) cases, where the overall profit is determined as a function of equipment sizes, stage cycle times and number of product batches. For this purpose, stage operations for each product are implicitly fixed by the solutions to the unit subproblems, as in recipes. In particular, state and control profiles, initial and final batch conditions, processing time requirements at each stage and batch sizes are fixed.

For simultaneous profit maximization (SM), reactor and column dynamic models are included in the design and scheduling formulation along with constraints to relate the initial condition at the column with the final condition at the reactor for a batch. This allows processing time in the reactor and column, state and control profiles for each product and batch sizes to be treated as variables. For all SM cases, the final condition of a batch at the reactor as well as the initial condition at the column are fixed at values corresponding to the solutions of unit subproblems in the sequential approach. The SM cases would

thus reflect improvement of a simultaneous approach over a sequential one, with some processing potential left to be exploited.

In simultaneous SM* cases, final condition of batches in the reactor as well as initial conditions in the column are also included as decisions. The overall problem is solved as one to reflect processing tradeoffs between the reactor and column operation, as far as sharing the "processing load" for. a product goes. In all cases, problems are subjected to the same horizon and production constraints.

$$\begin{array}{lll} \max & tl>_P profit(Vj, CTj, n») & \\ \text{s.t.} & \{CTj \leq H, \quad uij(t\backslash \quad t_{ij}, \quad B_i, \quad , z^f_{ij}, z^i_{ij}) & \text{(SQ)} \\ \max & \psi_{profit}(V_j, CT_j, n_i, u_{ij}(t), t_{ij}, B_i) & \\ \text{s.t.} & (CT_j \leq H, \quad z^0_{i,IV} = f(z^{R0}), \quad z^f_{ij}, z^i_{ij}) & \text{(SM)} \\ \max & \psi_{profit}(V_j, CT_j, n_i, u_{ij}(t), t_{ij}, B_i, z^f_{ij}, z^i_{ij}) & \\ \text{s.t.} & (CT_j \leq H, \quad z^0_{i,IV} = f(z^{R0})) & \text{(SM*)} \end{array}$$

All problems in each case are solved in the same order, starting with a constant operation in both the reactor and column and allowing general profiles to be included successively. Solution for a problem initializes the next one, in the order ROCO, R0C1, RICO and R1C1. Reactor and column subproblems are solved first to generate data for the SQ cases. These also provide initialization for problems ROCO with constant operations in both simultaneous cases.

### 3.2.3 Results

For all problems (ROCO - R1C1) profits are greatest for SM* cases and least for SQ cases. In addition, for all cases (SQ, SM or SM*) profits improve when optimal profiles are included in dynamic units for most problems.

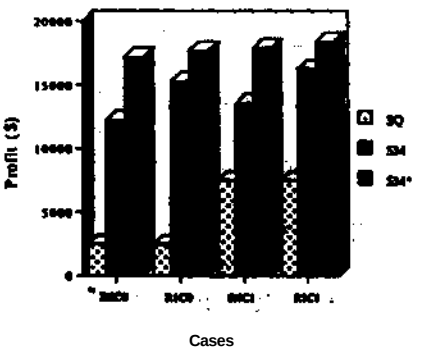


Figure 8: *Performance of cases for example 2.*

Results for reactor subproblems are compared in (Table 6). Final state for RO yields a starting binary composition in the column of (0.233,0.767). Problem Rl achieves the same starting composition in a time that is about 13 % less due to the transient relaxation of temperature profiles.

| Operation | *Uj* (hr.) | $*l_{rv}$ |
|---|---|---|
| Constant (RO) | 1.0000 | (0.233,0.767) |
| Dynamic (Rl) | 0.8765 | (0.233,0.767) |

Table 6: *Comparison of the reactor operations for example 2.*

The optimal temperature profile starts at a high temperature as only the first reaction is active in the beginning. As a result more C is favored in the beginning. As soon as a significant amount of P is formed, a low temperature prevents its degradation to waste G. Towards the end there is little time available for degradation via the third reaction, as a result the temperature rises gradually to convert C to P. Final state is thus achieved in a shorter time with a more intense operation. An increasing reflux profile similarly separates the specified size batch in a shorter time as compared to a constant operating level.

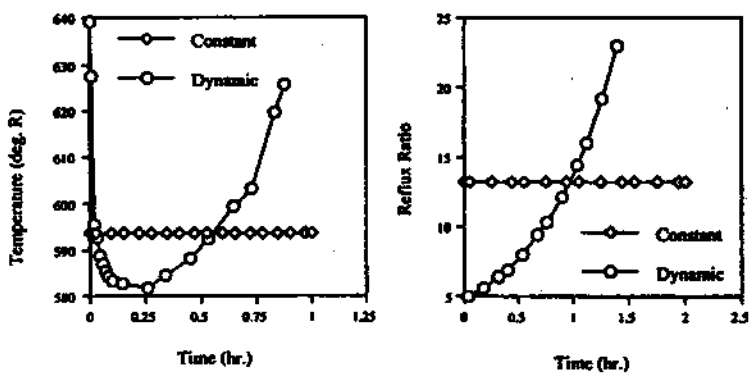


Figure 9: *Comparison of profiles in example 2.*

Table 7 shows processing time and batch size data from solving column subproblems with initial conditions determined by the solution of reactor subproblems. Also shown are profit values for various SQ cases. Reactor and column processing times for problem R0C0 are the largest although these were specified for the subproblems. Batches of purer products are smaller in size as all products are started with identical initial conditions and processed for the same time. Results must be compared keeping in mind that the processing times for dynamic units were specified at will.

Sequential profit maximization provides no advantage of speeding up the reactor operation (Rl vs. R0) when the column is the "bottleneck" stage. Time

reduction in the column (Cl vs. CO) however allows more batches of the same size to be processed in the available **horizon. As product 3** is **the most profitable,** 38 extra batches of it are accommodated corresponding to an increase of $ 5,037 in value.

| ,1 Prob. | *tl* (hr.) | t/v (hr.) | | | Batch size (lb.) | | | *1>profit* |
|---|---|---|---|---|---|---|---|---|
| W | *U.l* | *h,iv* | *t2JV* | *Hjv* | *Bi* | *B₂* | #3 | (*) |
| ROCO | 1 | 2 | 2 | 2 | **42.08** | 43.12 | 44.08 | 2,428 |
| RICO | 0.8765 | 2 | 2 | 2 | 42.08 | 43.12 | 44.08 | 2,428 |
| ROC1 | 1 | 1.448 | 1.447 | 1.449 | 42.08 | 43.12 | 44.08 | 7,465 |
| RlCl | 0.8765 | 1.448 | 1.447 | 1.449 | 42.08 | 43.12 | 44.08 | 7,465 |

**Table** 7: *Results of* ***sequential*** *subproblems (R0C0 -* ***RlCl).***

**The SM** cases **perform considerably better, gaining both from a simultaneous formulation as well as "free" processing time. In all of the SM cases, all products require processing in the reactor and column for the same time, allowing idle times for each product pair to remain only in recipe based stages. Final reactor states are constrained to provide initial conditions in the column that are identical with** the **SQ case, after the effect of the separator is accounted for.**

| Problem Id. | Time (hr.) | | Batch Sizes lb. | | | *Profit* |
|---|---|---|---|---|---|---|
| | *U.I* | *Ujv* | *B* | *B₂* | *3 | (*) |
| SMR0C0 | 0.89 | 0.89 | 32.08 | 33.18 | 34.19 | **12,189** |
| SMR1C0 | 0.69 | 0.69 | 28.05 | 29.09 | 30.03 | **15,114** |
| SMR0C1 | 0.89 | 0.89 | 33.97 | 35.07 | 36.07 | **13,481** |
| SMR1C1 | 0.69 | 0.69 | 29.25 | 30.29 | **31.23** | **16,169** |

**Table 8:** ***Results for SM cases.***

**Control profiles for both units suggest a more intensive operation where the reactor achieves final state specifications as soon as possible (0.89 hours with the best constant operating point and 0.69 hours with an optimal temperature profile) and the column maximizes the separated batch while operating for the same time. Because of a reduced time of 0.69 hours for the limiting bottleneck stages (reactor and column) with transient reactor temperature profiles (case R1C0 and R1C1), smaller batch sizes are more than compensated by increased number of batches that can be accommodated in the available horizon.**

**When specifications on initial column conditions are relaxed and included as decisions, all stage processing times reduce** to **0.5 hours. This situation corresponds to no slacks appearing anywhere in the schedule however for** a **more** general case it is expected **that** "free" processing **times would adopt** values corresponding to the longest processing in all recipe based units. This result could be useful in developing sequential strategies for very large scale problems.

Initial column conditions are better when a transient reactor temperature

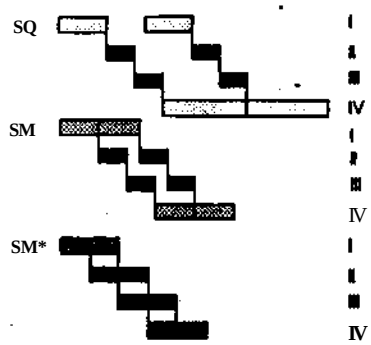


**Figure 10:** *Identical processing and slack times in example 2.*

| Problem Id. | Time(hr.) $U_i$ | $U_{jv}$ | Batch Sizes lb. $B_i$ | $B_2$ | $B_3$ | ^profit ($) |
|---|---|---|---|---|---|---|
| SM'ROCO | 0.5 | 0.5 | 21.75 | 22.62 | 23.40 | 17,138 |
| SM'RICO | 0.5 | 0.5 | 22.14 | 23.01 | 23.80 | 17,628 |
| SM'ROCl | 0.5 | 0.5 | 22.31 | 23.18 | 23.96 | 17,824 |
| SM'RICI | 0.5 | 0.5 | 22.70 | 23.59 | 24.38 | 18,321 |

**Table 9:** *Results for SAT cases.*

profile is allowed (0.227,0.773) than when the reactor operates at the best constant level (0.224,0.776). For both cases, upper bounds are active for the temperature profiles close to the end.

Transient column reflux profiles are able to extract bigger batches than when operating at the best constant reflux level. Processing times being the same for all SM* cases, profits differ marginally due to unequal batch sizes, and hence number of batches.

| Cases J | R0C0 | R1C0 | R0C1 | R1C1 |
|---|---|---|---|---|
| SQ | 0.09 | 0.13 | 0.07 | 0.10 |
| SM | 2.00 | 1.96 | 1.98 | 2.05 |
| SM' | 1.82 | 1.96 | 1.98 | 2.00 |

**Table 10:** *CPU seconds for solving example 2 using the NLP solver CONOPT through the GAMS modeling system on an HP 9000/700 workstation. Unit subproblems require 2.42 CPU seconds in total.*

It is worth pointing out that recipe based processes are generally operated with simple operating profile structures such as a constant operating level, that are arrived at by heuritics or crude experimentation. The incentive for allowing transient profiles can be judged by comparison with a particular recipe. The

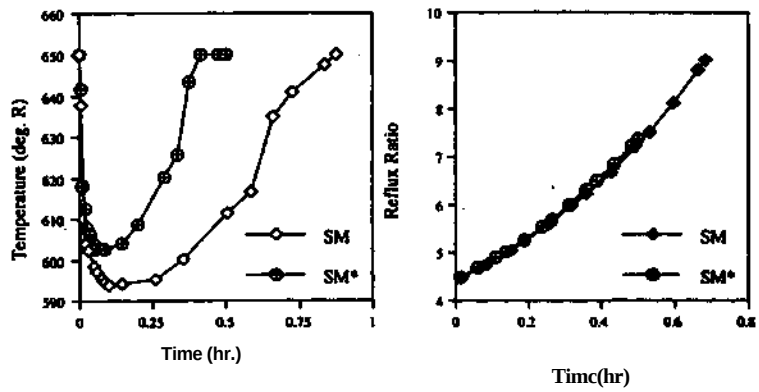


Figure 11: *Profiles for SMR1C1 and SWRICI cases.*

ROCO cases here represent the best that can be achieved with recipes of one specified structure *i.e.* constant operation, as .their solution employs dynamic models of the process. The improvement over these cases is therefore the smallest over any constant operation recipe.

# 4 Inventory Considerations

The impact of operating profiles through processing time and batch size decisions in resolving inventory and production tradeoffs is explored next. For this purpose the formulation in [10] is utilized. This formulation considers ZW policy, where storage costs can be related to final levels of each product. These levels build up during the part of the campaign dedicated to the production of the particular product (T<) and are depleted by constant market demands. If the number of batches of each productitis^ufficiently large, storage costs are related with appropriate cost co-efficients (//;) to the area of *inventory triangles* (figure '12)*constructed by approximating the production as continuous.

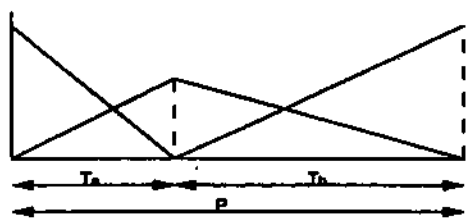


Figure 12: *Inventory triangles - two product case.*

$$\psi_{inv} = \sum_i \mu_i (Q_i/2)(P - T_i) \tag{14}$$

The production targets for the horizon are divided equally over a number of identical production cycles of single product mode and duration $P$ each. If costs are associated with changing over from one product to another then operating with a large number of cycles would not be profitable. A tradeoff therefore exists between the number and length of these cycles. Larger cycles would require greater inventory costs but reduced changeover costs. Smaller cycles on the other hand lead to large changeover costs with low storage costs.

## 4.1 Formulation

The model for inventory considerations in [10] considers the following formulation.

$$\min \quad \psi_{cost}(P, T_i, NC)$$

$$\text{s.t.} \quad Vjt\text{-}SijBi \quad V^*,j \tag{15}$$

$$* = |j'' V * \tag{16}$$

$$\sum_{k=1}^{N_p} NPRS_{ik} = rii \quad Vi \tag{17}$$

$$J2 \wedge PRS_{ik} = n_k \quad Vk \tag{18}$$

$$Ti = \left( nfitf + \sum_{k=i}^{N_p} SL \wedge . NPRSik \right) J, \quad j' = J \tag{19}$$

$$\sum_{i=1}^{N_p} \left( n_i t_i + \sum_{k=1}^{N_p} SL_{ikj} NPRS_{ik} \right) < P \quad Vj \tag{20}$$

$$SLikj + t_{kj} = t_{i,j+i} + 5L < fcj+i \quad Vt.j.A;; \quad j \neq J \tag{21}$$

$$NPRSu = n_{i-1} \quad Vt \tag{22}$$

$$Hq_t = PQi \quad Vt \tag{23}$$

$$H/P = NC \tag{24}$$

$$Vj \geq 0, ni, Bi \geq 0, \; NPRS_{ik} \geq 0, P \geq 0$$

where $P$ is the duration of each cycle,

i T< f? **is the part of $P$ dedicated for product t**

$NC$ are the number of cycles (relaxed from integers),

$q_i$ is the amount of product t to be produced in each cycle.

Equation( 16) gives the number of product batches in each cycle. Equation( 19) gives the time dedicated to the production of each product at the last

stage. The equality in equation( 22) specifies single product campaigns. Equations( 23) and ( 24) ensure that the horizon and production targets are divided equally over the *NC* production cycles.

Although a rigorous MILP solution method is suggested for this problem in [10], for. the purpose of this work the number of cycles variable is relaxed from taking integer values. Our intention here is to assess the role of dynamic process modelling in improving the inventory planning problem for which reason the issue of rounding off these relaxed integer variables will not be considered. Since the model is solved to meet fixed production targets, a revenues term in the objective would not be required. Instead incentive is provided for achieving the targets soon, through an operating cost term proportional to the production horizon which is treated as variable. Equipment costs are not included in the objective as equipment sizes were found to be insensitive to operating decisions when the amount of initial load to the column is held fixed. The overall cost objective to be minimized with process operating decisions is of the form:

$$\psi_{cost} = \underbrace{\sum_i \mu_i (Q_i/2)(P - T_i)}_{\psi_{inv}} + \underbrace{\gamma NC}_{\psi_{change}} + \underbrace{\sum_j OC_j P}_{\psi_{op}} \tag{25}$$

The formulation is used to explore the impact of processing decisions in inventory consideration for example 2.

## 4.2 Solution Strategy

Processing time and batch size data from the solution of unit subproblems is used to minimize the cost objective for the sequential solution (SQ cases). The simultaneous approach includes unit models within the cost minimization allowing processing times and batch sizes to be determined more sensibly, with fixed (SM cases) and relaxed (SM*) reactor final conditions. The problems are solved successively with transient relaxation of reactor and column control profiles, as in previous cases. However, one of the SM cases (SMR1C1) had to be initialized with the solution of case SMR0C0.

## 4.3 Results

All problems give reduced costs when operating profiles are considered as decisions in the minimization. Again, SM* cases perform best being the most general and relaxed formulation out of all studied. Sequential solutions do not exploit the tradeoffs between processing decisions and give highest costs for all cases.

For the SQ cases processing time and batch size data from the solution of unit subproblems is used (Table 7). Allowing a dynamic temperature profile in the reactor provides no improvement when the column introduces a bottleneck in time. Cases SQR0C0 and SQR1C0 perform identically as a result even though

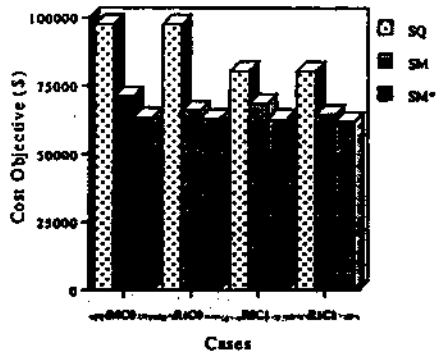


Figure 13: *Results for example 2.*

| \\ Cases SQ | ROCO | RICO | R0C1 | R1C1 |
|---|---|---|---|---|
| Vw($) | 97,478 | 97,478 | 80,231 | 80,231 |
| *1>inv* ($) | 47,769 | 47,769 | 34,791 | 34,791 |
| *Ipchange* ($) | 35,000 | 35,000 | 34,791 | 34,791 |
| $1>O_p$ ($) | 14,708 | 14,708 | 10,648 | 10,648 |
| *P* (hr.) | 191.0 | 191.0 | 139.1 | 139.1 |
| H (hr.) | 6,685.5 | 6,685.5 | 4,840.3 | 4,840.3 |
| ATC | 35 | 35 | 34.8 | 34.8 |

Table 11: *Results for SQ cases.*

the reactor processing time is reduced to achieve the same final state. The inventory and changeover costs are unbalanced only for these two cases, all other cases give these two terms in the objective to be equal. Case SQR0C1 shows an improvement over these cases in all the three objective terms. A reduction in the column processing time allows a slight increase in production per cycle with cycles of much shorter duration. As a result the production horizon is also reduced. In case SQR1C1, the reactor profile is also allowed although this only speeds up the process unnecessarily and provides no other benefit.

Minimizing the costs simultaneously with a specification on the final state of the reactor corresponding to that in the SQ cases leads to further savings due to a more general formulation. All processing decisions are resolved as in the previous cases for scheduling and are not presented again. Both the reactor and column processing times take equal values, not speeding up the process in any unit beyond what is required. For the SMR0C0 case, fewer cycles than in SQ cases are required. This means the production demand to be met in each cycle will be higher. The batch sizes for each product are also smaller implying a greater number of batches of each would be required. A higher production rate is however made possible by restricting the processing time in the column at 0.89 hours thus increasing utilization in the more efficient region. With an operating profile in just the reactor (temperature), its final state is achieved in

| Cases SM | ROCO | RICO | R0C1 | R1C1 |
|---|---|---|---|---|
| Vw ($) | 70,688 | 66,184 | 68,522 | 64,702 |
| * . . (S) | 31,094 | 29,315 | 30,240 | 28,725 |
| *1>chanQe*($) | 31,094 | 29,315 | 30,240 | 28,725 |
| *1>op*($) | 8,449 | 7,553 | 8,040 | 7,252 |
| P (hr.) | 124.3 | 117.1 | 120.9 | 114.8 |
| ff (hr.) | 3,864.2 | 3,418.0 | 3,654.8 | 3,286.1 |
| *NC* | 31.1 | 29.3 | 30.2 | 28.7 |

**Table 12:** ***Results for SM cases.***

**a time that is less and limits the column operating time. As a result batches are slightly smaller giving a higher production rate in a smaller horizon.**

**An operating profile in just the column (reflux) performs better than case SMR0C0 but not as well as SMR1C0. This is because the reactor takes a longer time (0.89 hrs. vs. 0.69 hrs.) with a constant temperature operation to realize the final state specification. The benefit of a profile in the column then is to extract a larger batch in the less efficient part of its operation. As a result batches are bigger in size leading to a slightly higher production rate. The horizon, length and number of cycles all reduce correspondingly. Finally in SMR1C1, both the profiles contribute to improving production rate. The demand met in each cycle goes up with a reduction in their duration.**

| Cases SM* | ROCO | RICO | R0C1 | R1C1 |
|---|---|---|---|---|
| *i>co»t* ($) | 63,539 | 62,930 | 62,672 | 62,077 |
| * . . ($) | 28,260 | 28,016 | 27,912 | 27,673 |
| *^change* ($) | 28,260 | 28,016 | 27,912 | 27,673 |
| $f/f_{op}$ ($) | 7,018 | 6,897 | 6,847 | 6,730 |
| *P* (hr.) | 112.8 | 111.9 | 111.5 | 110.5 |
| i/ (hr.) | 3,181.0 | 3,131.3 | 3,112.3 | 3;059.8 |
| iVC | 28.2 | 28.0 | 27.9 | 27.7 |

**Table 13:** ***Results for SAT cases.***

**Finally when final state specifications for the reactor operation are dropped, overall costs reduce slightly. A transient relaxation of operation in the reactor and column reduce these costs further but only marginally.**

# 5 Conclusions

**Batch operations provide many interesting tradeoffs between various aspects of production. A detailed description of these is presented in [10]. At the heart of batch operations lies the process. In particular, processing times for products at different stages play a critical role in limiting the benefits of accounting for**

these tradeoffs.

Although the work here concerns tradeoffs between equipment and batch size decisions vs. production span for a limited class of batch operations, examining these tradeoffs with more detailed models is a potentially lucrative proposition. In view of its reasonable computational requirements, the collocation method embedded in (NLP1) in addressing process decisions is very promising.

This work relies on many simplifying assumptions that can limit its scope, as well as the acceptability of the solution. For instance all integer variables, such as the number of column trays, the number of batches and product pairs, are either fixed or treated as continuous. Equipment sizes generally come in discrete sizes. In this light, the solution provided is only a preliminary one that must be refined further. Extensions with integer variables would necessitate the use of MINLP methods that require added computational load.

It would be interesting to consider process decisions in relation with plant superstructure, unit task assignments etc.

Processing considerations can transform a situation in less expected ways. For instance, in problems with ZW policy in this work, the processing times for all products that are left as decisions are decided with the same value. This implies that all products become identical as far as stage requirements go. The difference only appears in the operating policies. It is also expected that at least the stages with "free" processing times would be bottlenecks in the ZW context, unless there are high costs associated that prevent this. For the examples in this work ik becomes very simple to determine the schedule which now becomes sequence independent even for the ZW case. This however will not usually be true when recipe based stages process the products for an unequal duratiori^pr when unequal cleaning and transfer times exist for different products. Finally, dynamic optimization is expected to be most critical in units that form bottlenecks. Depending on how sensitive a bottleneck operation is to dynamics, extra equipment at that stage operating in or out of phase could be avoided by considering optimal dynamic processing.

The assumption of perfect dynamic models inherent in this work is a very strong one. Most of the challenge in including dynamic process considerations would rest on how reliable the models are. Deriving appropriate models for different stages or appropriate techniques to deal with imperfect models will be a critical step in adding confidence to the results of such integration. This is the focus of our future work.

Nevertheless, this paper shows dynamic process considerations can contribute significantly to increase profitability through reduced investments or increased returns by addressing the problem at a critical level. Also, collocation over finite time elements can serve to include dynamic process considerations very efficiently in planning, scheduling and other strategic levels.

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# A Data for example 1

- Stage I Dynamic Reactor
  - Reaction

    $A \longrightarrow B^*$ desired
    $A \longrightarrow C$

- **Mass balances**

$$\dot{x}_B^i = +\alpha_i u_i(t)^{\beta_i} \qquad \text{Vz}$$
$$\dot{x}_A^i = -\left(\alpha_i u_i(t)^{\beta_i} + u_i(t)\right) \qquad \text{Vi}$$
$$x_A^i + x_B^i + x_C^i = 1 \qquad \text{Vi}$$

- **Reaction parameters**

| $i$ | 1 | 2 | 3 |
|---|---|---|---|
| $a_t$ | 2 | 2 | 3 |
| ft | 0.5 | 0.4 | 0.5 |

- **Stage II and III**

*i,//= 0.4 Vi

*UJII* = 0.6 Vi

- **specifications**

Reactor load = 100 units; z£$_7$ = (1,0)

$$ij > Pi = 60CT/ + 40CT// 4- 40CT///$$
$$s.t. Vj = 150/. \quad Vj, \quad Qi = 4800 \quad Vi,$$
$$\psi_{P2} = 300V7^{09}\ 4- 230V\}^{0}/^{8} + 210V?/?^{5}$$
$$s.t. Q_i = 4800/6. \quad Vi, \quad CTj \leq 200 \quad Vj$$
$$\psi_{P3} = 3(\mathrm{E}_{i}\, n_i B_i)$$
$$s.t. Vj = 150/. \quad Vi, \quad CTj \leq 200/\text{irs}. \quad \forall j,$$
$$\psi_{P4} = \psi_{P3} - 0.1(\textstyle\sum_i 100 n_i) - \psi_{P1} - \psi_{P2}$$
$$s.t JQi \leq 10000 \quad Vi$$

# B Data for example 2

- **Stage I Dynamic Reactor**

- **Reaction**

$$A + B \xrightarrow{k_1(T)} C \qquad k_x(T) = (5.9755 \times 10^{9})e^{(\frac{-12000}{T})}$$
$$C + B \xrightarrow{k_2(T)} P + E \qquad k_2(T) = (2.5962 \times 10^{12})e^{(\frac{-15000}{T})}$$
$$P + C \xrightarrow{k_3(T)} G \qquad k_z(T) = (9.6283 \times 10^{15})e^{(\frac{-20000}{T})}$$

— **Material balances**

$$\dot{w}_A = -ki(T)w_A w_B$$
$$\dot{w}_B = -ki(T)w_A w_B - k_2(T)w_B w_C$$
$$\dot{w}_c = +2hi(T)w_A w_B - 2k_2(T)w_B w_- k_3(T)w_C w_P$$
$$\dot{w}_E = +2k_2(T)w_B w_C$$
$$\dot{w}_P = +k_2(T)w_B w_C - 0.5k_3(T)w_C w_P$$
$$\dot{w}_G = +l.5k_3(T)w_P w_c$$
$$WA + WB + we + WE + wp + WG = 1$$

- **Stage II and III Recipe Based**

$UJJ = 0.5$ Vi
*i,///=0.5 Vi

- **Stage IV Dynamic Distillation Column**
  - **Mass balances**

$$\dot{S} = -\frac{V}{R+1},$$
$$\dot{x}_b^1 = -\frac{V(x_b^1 - x_d^1)}{(R+1)S},$$
$$\dot{x}_b^2 = -\frac{V(x_b^2 - x_d^2)}{(R+1)S},$$
$$x_b^1 + x_b^2 = 1, \qquad x_d^1 + x_d^2 = 1,$$

— **Underwood's Correlation**

$$\frac{\alpha_1 x_b^1}{a\text{\—}7} + \frac{\alpha_2 x_b^2}{\text{QI2—7}} = 0,$$
$$\frac{\alpha_1 x_d}{a\ ,\ _\ 7} + \frac{\alpha_2 x_d}{0\ 2\ -\ 7} = R_{min} + 1$$

– **Gilliland's Correlation**

$$v - 1 - exv\left[\frac{(1+54.4X)(X-1)}{(11+117.2X)\sqrt{X}}\right],$$
$$X = \frac{R - R_{min}}{R+1},$$
$$y = \frac{N - N_{min}}{N+1}$$

- **Hengstebeck-Geddes' Equation**

$$\frac{x_d^2}{x_b^2} = \left(\frac{\alpha_2}{\alpha_1}\right)^{N_{min}} \left(\frac{x_d^1}{x_b^1}\right)$$

- **Purity Constraints**

$$\frac{\int_0^{t_f} \frac{x_d^1 v}{R+1} dt}{\int_0^{t_f} \frac{v}{R+1} dt} = \bar{x}_d^i \qquad \forall i$$

where 5 is mass in the column
$R$ is reflux ratio,
$x^{l}_{d}$ is distillate composition for component 1,
$x\backslash$ is reboiler composition for component 1,
$e^{*}2$ is relative volatility,
7 are Underwood roots,
$\bar{X}d$ final average composition of ditillate.

- **Specifications**

$z?j$ = (0.30303,0.69697)
$550H \leq T \leq 6S0R$

Column vapor rate = $300 *_{h} = \wedge$ Number of trays = 10
$0 \leq R \leq 25$
Intial $Ioad5_0 \leq 200$
$CTj \leq 200$
$Qi \geq 1200$ Vt
$\psi_{profit}$ = $(2.2niBi + 2.5n_2JB_2 + 3JI3B3)$
$-(1.25V_1^{0.7} + Vj^{-B} + 1.1V^{\wedge 5} + 1.5V?^{8})$
$-(12CTi + 8CT_2 + 8CT3 + 16CT_4)$ \$

- **Inventory Problem**

$Qi$ = 48,000 Vi
$\wedge$ = 0.004,0.005,0.0066
$OCj$ = 0.6,0.4,0.4,0.8
7 = 1000
$15 \leq NC \leq 35$