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Dynamic Optimization in Planning Under Process Model Uncertainty

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EDRC 06-237-97
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November 26, 1996

Abstract

Planning for multi-product batch plants involves decisions for facility design, product scheduling, inventory control etc. These are usually addressed for recipe based processes with fixed stage processing times. There is significant benefit in incorporating detailed dynamic process models while planning, and addressing the overall problem simultaneously (Bhatia and Biegler [1]). It thus becomes desirable to have sufficiently accurate process models, or develop methods that deal with process model uncertainty.

This work addresses dynamic processing and planning decisions simultaneously for multi product batch plants, now with uncertainty in process parameters. Instances of uncertain parameters are used to construct planning scenarios that are addressed through a multiperiod planning formulation. Dynamic processing under uncertainty is addressed via a closed loop state feedback based correction strategy. Control parameters in the closed loop implementation of processing decisions are then determined in an open loop manner, and treated as invariant design variables in the multiperiod problem formulation.
1 Introduction

Batch processing is intrinsically dynamic and provides transient operating freedom. This allows improved profitability, when processing decisions are incorporated simultaneously during planning. Planning includes facility design, batch scheduling, production and inventory planning. However, when process parameters vary or are not precisely known, an integration of processing decisions in planning must consider this uncertainty.

For the overall processing and planning problem, uncertainty in the processing subproblem transcends to uncertainty in planning. Processing under model uncertainty is better addressed through closed loop methods, that rely on monitoring a process and taking remedial measures. One such approach is the updating of an input profile via state feedback and correction. In contrast, planning involves broad decisions that are taken once every planning period. In this sense, planning decisions under uncertainty are usually performed in an open loop manner. This difference makes it challenging to develop a unified approach that addresses processing under uncertainty and production planning. This paper proposes one such approach. The main idea is to discretize the dynamic process models, and include them along with the planning constraints through a multi-period planning problem. In this manner, all decisions can be made in an open loop sense, with closed loop correction incorporated in the formulation.

The paper is organized as follows. Process integration in planning is discussed first. The problem is presented in section 2, followed by the proposed approach. Problem formulation and the model are developed in section 3. These include a novel treatment for addressing constraints on the input policies. The approach is then demonstrated for a one dynamic stage example involving an uncertain operation for one product, in section 4. Uncertainty is then extended to a multiple product formulation. For this case, a more efficient general framework for formulating the problem is also presented. Next, a two dynamic stage example with uncertain operations for all products is discussed in section 5. Finally, directions for future work are identified.

Dynamic Processing and Planning

Market driven specialty chemical production is often addressed in the flexible batch operating mode. At the heart of batch operations lie dynamic processing units, providing transient processing flexibility. However, planning often considers batches along recipes with fixed processing times and operating strategies, e.g. Voudouris and Grossmann[22], Birewar and Grossmann[2] and [3]. This is attributed to (i) a lack of accurate process models, (ii) large development time for process models of sufficient detail and (iii) complexity of the resulting overall problem. There is also little incentive in pursuing detailed process models in view of short product lives. However, process interaction in planning can be significant for dynamic units.

In a recent work (Bhatia and Biegler[1]), processing tradeoffs are explored in design, scheduling and inventory planning, for a special class of batch operations, i.e. flowshop plants with zero-wait (ZW) and unlimited intermediate storage (UIS) transfer policies with one equipment unit per stage. Dynamic processing decisions are resolved by parameterizing the dynamic process models through collocation on finite elements. This transforms the infinite dimensional optimal control problem for processing, which requires solution of a system of differential and algebraic equations, to a finite dimensional pure algebraic system. Combinatorial scheduling issues are simplified by the class of problems considered, using the formulations of Birewar and Grossmann[3] and Voudouris and Grossmann[22]. Their formulation expresses the performance of the planning problem in the design objective, through a closed form. The overall problem is then posed as an NLP of the form (M1).
\[
\begin{align*}
\max_{z,u,v} & \quad r^f(z,u,v;\theta) \\
\text{s.t.} & \quad f^f(z,u,t;\theta) = 0 \\
& \quad h^p(z,u,v;\theta) = 0 \\
& \quad z,u \in Z, v \in P, e = \{e\setminus\theta\} \tag{M1}
\end{align*}
\]

The profit objective function \(r^f\) is maximized subject to constraints \(f^f\) for the discretized dynamic stage operations, and \(h^p\), for the planning problem. Variables \(z,u \in Z\) are parameters in the discretized process models for state and control variable profiles. Variables \(v \in P\), are planning variables such as equipment design and scheduling decisions. Problem parameters consist of \(\theta^f\) for stage operations and \(\theta^p\) for the planning problem. Often these parameters are uncertain or subject to change. These two problems are coupled and addressed simultaneously through (M1).

Processing decisions include stage processing times, input variable profiles, and final batch states in dynamic stages. Each of these directly influence the planning problem. Processing times affect scheduling and sequencing of products and final batch states affect the number of product batches. In [1], improved planning with dynamic input policies for a three stage (one dynamic reactor) problem reflects higher and more time efficient product conversions than operating with constant input policies. The overall profit in this example improves by about 16\% for ZW and 11\% for the UIS policy, when dynamics are considered in the reactor.

With more than one dynamic stage, processing times change and process loads shift among units to provide efficient schedules with reduced idleness. In a four stage example, with batch reaction and distillation modeled through dynamic process models, a 7\% improvement in the planning objective is realized. Similar effects improve an inventory planning objective by 2.3\%. Considerable savings can thus result from an integration of processing decisions in planning.

The previous work demonstrates significant motivation to integrate processing and planning decisions for a special class of problems, with totally deterministic process models. However, plant model mismatch, both parametric and structural, is not considered. Consequently, implementation of these processing decisions for slightly different parameter values in an actual situation could give sub-optimal and perhaps infeasible performance. This motivates addressing uncertainty in the process models when processing and planning decisions are addressed together.

The problem of design and processing under uncertainty is recently reviewed by Pistikopoulos [17]. In this area, issues such as feasibility, flexibility, controllability and operability are important at the design stage. In a broad sense the area covers (i) a feasibility test that requires operational constraint satisfaction over a considered uncertain parameter hyperspace, (Halemane and Grossmann[9]) (ii) the notion of flexibility and flexibility index associated with a given design that quantifies the portion of the uncertain hyperspace that passes the feasibility test, (Swaney and Grossmann[18],[19]) and (Hi) integration of design and operations where tradeoffs between flexible operations and fixed design costs are explored based on these previous concepts, (Grossmann et al [8]).

A limitation of flexibility analysis is that it relies on feasibility at many uncertain points in the uncertain hyperspace, leading in turn to large multiperiod NLP or MINLP models. Special techniques, that work with critical parameters and their combined instances as well as special algorithms that solve subproblems iteratively are combined to address design and operations under uncertainty. Such problems rely on the
solution of multiperiod optimization problems at each iteration* that can be large due to repeated model instances for each uncertain scenario linked via a set of invariant design variables.

## 2 Problem Description and Approach

This work incorporates process parameter uncertainty in integrating dynamic processing and planning decisions. The problem can be stated as a simultaneous incorporation of closed loop dynamic processing decisions under uncertainty, in the planning of multi-product batch plants. We address this problem through multi-period strategies that account for uncertainty and a set of control decisions.

Uncertainty is considered in process parameters as instances of probable values and not in the planning parameters such as market demands. However, instances of processing parameters lead to different planning scenarios. In this manner the approach could be easily extended to include uncertainty in planning parameters. Different scenarios are considered through a multi period planning problem, where a weighted planning objective is improved. In addition, a robust implementation for the input policy in the face of uncertainty, is desired.

### 2.1 Background and Discussion

Grossmann and co-workers have integrated aspects in planning, excluding processing decisions (e.g. Voudouris and Grossmann[22]). They, and others, have also addressed uncertainty in planning (e.g Varvarezos et al[21], Pistikopoulos[17]). Uncertainty in dynamic processing at single batch stages has also been addressed (e.g. Terwiesch and Agarwal[20]). For continuous operations, planning with uncertain processing conditions has been addressed (e.g. Morari and Perkins[15]). Ierapetritou and Pistikopoulos [10] address batch plant design with uncertainty in processing time and size factors in addition to market and production uncertainty without any detailed process models. Chiotti at al [5] address uncertainty in process parameters via posynomial models in a multiperiod formulation with adaptive operating policies. Also, Mohideen et al[14] integrate closed loop performance in the design of dynamic systems under uncertainty.

Open loop techniques require a representation of uncertainty. This is either probabilistic, where uncertain parameters are treated as stochastic variables with known probability distributions, or deterministic, where parameters are assumed to take a set of values within certain bounds. Operating strategies are then resolved with suitable objectives that reflect, in some weighted sense, relevant performance criteria. A deterministic representation of uncertain space can be treated as a grid, each point therein representing a probable scenario. This becomes comparable to a multiperiod design formulation (Varvarezos et al.[21]) often used in planning.

Closed loop techniques address uncertainty directly, relying on some means of estimating the current situation and then taking appropriate corrective action. These techniques are preferred, when convenient, over resolving processing conditions for every possible instance of uncertain parameters in the operation at a processing stage. For instance, initial batch state uncertainty can be treated by on-line correction of nominal profiles. This mitigates the effect of mismatch and reduces the need for a detailed uncertainty description in terms of probability bounds or functions.

One such method, in processing, is on-line re-optimization (Eaton and Rawlings[6]), where current state estimates are used to optimize the remaining part of the profile successively. This approach could serve our purpose, if feedback aspects of the profile can be conveniently represented (parameterized) in the planning problem. A more general approach is to correct the nominal control profile through linear state feedback laws (Terwiesch and Agarwal[20]). In aerospace applications similar techniques are used for correcting the
path of space vehicles with limited on-board computing (Pesch[16]). The feedback law approach permits profile implementation and planning to be addressed together, and is discussed next.

2.2 Proposed Approach

In an integrated processing and planning formulation, uncertainty in process parameters translates to planning under uncertainty. It is clear that planning and processing problems require different approaches for dealing with uncertainty. A unified approach that addresses both aspects requires special effort.

First consider the simultaneous processing and planning formulation in Bhatia and Biegler [1], with no uncertainty in processing parameters. In a flowshop plant, each product \( t \in I \), \( I = \{1, \ldots, N_j\} \) is processed through the stages \( j \in J \), \( J = \{1, \ldots, N_j\} \) in an identical flowshop sequence. Stages modeled by systems of differential and algebraic equations (DAE) are in the set \( Jd(C) \), other stages process along fixed recipes. Dynamic operations are discretized using Orthogonal Collocation over finite time elements. Indices \( I \) and \( m \) are reserved respectively for time elements and collocation points therein. A general profit function of stage cycle times \( (CT_j) \), equipment parameters \( (V_j) \) and production capacities \( (Q_i) \) is maximized subject to the discretized dynamic process models, equipment sizing and scheduling constraints.

\[
\begin{align*}
\max_{x,u} & \quad \psi(CT_j, V_j, Q_i) \\
\text{s.t.} & \quad \begin{cases} \\
& \begin{aligned}
z^L & \leq z \leq z^u \\
u^L & \leq u \leq u^u \\
4 = f(z^{'}, h^{'}) & W_i J J^* h^{'J} = J - 1 \end{aligned} \\
B_i = f(z^{'}, h^{'}) & V_i J = \Pi J, \\
V_i, & V_i, 3, J_t J_d, 1^\text{stin} - \\
V_i & =
\end{cases} \\
& \begin{aligned}
n_i & = Y_{i,i} NPRS_{ik} = m \\
& = Y_{i,i} NPRS_{ik} = n_i \\
& \leq & NPRS_{ik} \leq n_i - 1 \\
CT_j & = \sum_{t=1}^{n_j} \left( n_i t_{ij} + \sum_{k=1}^{n_j} S_{ikj} \right) NPRS_{ik} V_j \\
CT_j & \leq H \\
SL_{ikj} + t_{kj} & = t_{i,j+1} + S_{ikj+1} V_{1,fc,j;j<Jv} \\
V_j & \geq 0, n_i, B_i \geq 0, NPRS_{ik} \geq 0, U_j \geq 0, S_{ikj} \geq 0 \end{aligned} \\
\end{align*}
\]

Variable \( U_j \) is the operating time for the \( ij \) operation. State variables \( z^L \) and \( z^u \) represent batch states at the beginning and end of the \( ij \) operation. Variables \( n_i \) and \( B_i \) represent the number and size of product batches respectively, \( NPRS_{ik} \) is the number of pairs of products \( t \) and \( k \) in the optimal processing sequence for ZW policy and \( SL_{ikj} \) is the slack time enforced at stage \( j \) when products \( t \) and \( k \) are processed successively in ZW.

With discrete uncertainty in processing parameters, different scenarios similar to the one in M2 occur for the planning problem. Here dynamic operation under uncertainty is addressed through a closed loop correction strategy. A nominal input profile is corrected on-line based on deviations in the observed state.
profiles from the nominal state profile. This correction uses a linear time varying feedback law, relating observed state deviations and required input deviations, through a profile of dynamic correction gains. This form allows closed loop processing of dynamic systems under uncertainty. Correction can be imposed as additional algebraic constraints. This still leads to a differential algebraic (DAE) form for the resulting closed loop dynamic system, which can be discretized and included in the planning problem as before. Processing decisions are now addressed via the discretized correction gain parameters, instead of the input profile parameters.

The different planning scenarios that result from combinations of uncertain parameter instances are treated through a multiperiod planning formulation. Process models, for each uncertain product stage operation are included along with the multiperiod planning formulation resulting in a large overall NLP problem. This approach allows processing decisions under uncertainty to be addressed simultaneously with decisions from the realm of design, production planning and scheduling, within one formulation.

In this manner, our operating policies are addressed via open loop parameters, and a unified approach that includes dynamic processing under uncertainty and planning is made possible. With a focus on implementation of processing decisions, if it is hard to identify the specific uncertain scenario at hand then a practical approach would be to treat processing decisions as the invariant design variables that do not change across periods. This corresponds to the case with robust input policies. However, if it is possible to identify the scenarios perfectly then a better approach would be to implement specific processing decisions in each period. This corresponds to a perfect information scenario. Clearly, the perfect information scenario is an ideal situation that is hard to realize and the robust input approach, though practical, is conservative. This motivates the development of a practical approach that performs better than the robust input approach.

In our proposed robust correction approach, closed loop implementation parameters for processing decisions are treated as the invariant design variables. These provide the desired implementation advantage in the face of uncertainty while accounting for uncertainty at the same time.

Consider Figure 1, where case PI corresponds to a perfect information scenario. The set of invariant design variables include only the facility design variables (V)). Case RI corresponds to improving each planning scenario subject to one robust input policy for all periods. Here, parameters in the dynamic input policy (u) are treated as design variables. The proposed feedback correction approach lies somewhere in between the two.

In the robust correction approach (Case RC), input profiles are not included directly as decisions. Instead, discretized closed loop expressions for a corrected policy are included for each period, as a function of the state and correction parameter profiles z and K. The feedback control parameters dictating this correction are then treated as invariant across each uncertain period. This shifts the implementation of processing decisions from the input operating policies to the correction parameters, offering a robust implementation advantage under uncertainty. Moreover, processing profiles can still vary across periods to improve the performance in each uncertain scenario.

3 Problem Formulation and Modeling

The overall problem formulation and modeling aspects are presented in this section.
3.1 Multi-period Planning Formulation

The overall dynamic processing and planning formulation presented in [1] is a non-convex NLP of the form (MI). In this work uncertainty is introduced in processing parameters, in terms of discrete instances. These combine to make different planning scenarios that are treated as the $p$ periods in the multi-period design formulation, of the form (MP).

$$\max_{x_p, u_p, v_p} \sum_p \omega_p \psi_p(x_p, u_p, v_p; \theta_p)$$

s.t. $h^p_p(x_p, u_p, v_p; \theta_p) = 0$ \quad $V_p$

$\hat{h}_p^p(x_p, u_p, v_p; \theta_p) = 0$ \quad $V_p$

$\ast, u \in Z, v \in P, 0_p$ \quad (MP)

Constraints $h^p_p$ and $bP_p$ model processing and planning aspects respectively and are included for each planning period. Operational constraints $\hat{h}_p^p$ in each period $p$ include the discretized differential and algebraic equations of the dynamic process models, for different process parameter instances.

3.2 Closed Loop Process Modeling

We now include closed loop dynamic process models for the stage operations in the multi-period planning formulation. The state feedback based corrected input profile is of the algebraic form in equation (1).

$$u(t) = \tilde{u}(t) + K^T(t)6z(t) \quad (1)$$

Here $\tilde{u}(t)$ is a reference input trajectory (e.g. from the RI case), that is not necessarily nominal, $K(t)$ is the matrix of correction gains and $6z(t)$ are deviations in the state profile vector from the reference state trajectory vector, $Sz(t) = z(t) - \bar{z}(t)$, for any uncertain operation. This form can be discretized in a manner
similar to other algebraic equations and included as constraints at each point in the collocation mesh. This results in constraints of the form in equation (2).

\[ u_0(t_{lm}) = u(t_{lm}) + K_f \delta_z(0) \quad V_0 \in O_{ij}, t_{f n} \]

(2)

The correction expressions are imposed at each discretized point in time. Index \( o \), corresponds to a member process operation in the set \( O_{ij} \) of all operations for the processing of a product \( f \) in stage \( i \), which involves uncertainty. In addition, the reference input and state profiles \( (u, z) \) though decisions, must be consistent with the process dynamics. For this purpose the dynamic model corresponding to the reference operation needs to be included with closed loop models of other operations in the overall formulation.

Since we seek an implementation strategy that remains robust in the face of uncertainty, constraining the implementation parameters to be equal in all models is not enough. Processing times for all \( f_j \) operations must also be equated in order to coordinate input profiles. The reference profile must also last an equal duration as the operations it is used to correct. This permits a convenient formulation of correction equations at collocation points.

\[ t = i \quad V_0 \in O_{ij}, V \in O_{ij} \]  

(3)

Different situations can be modeled as special cases of the overall multiperiod planning formulation. These are used to evaluate the proposed approach and are modeled by including additional constraints in the overall problem. The cases correspond to (i) Perfect Information, (ii) Robust Input and (iii) Robust Correction.

Perfect Information: This corresponds to the case where it is possible to resolve the uncertainty in processing parameters before starting a run. It is assumed that the processing parameters do not change during a batch run or from one batch to another during any planning horizon. If process parameters change across batches processed at different times in the campaign, such as an initial condition dependent on the season or source, then a multiperiod formulation is still appropriate for design. Consider problem \( (AfPl) \).

\[
\max_{z_p, \psi_p} \sum_p w_p \psi_p
\]

s.t.  

\[ h_p(z_p, u_p, v_p, O_{ij}) = 0 \]

\[ V_j \in D \]  

(\( MPI \))

In the perfect information case, only equipment design decisions \( (V_j) \) remain invariant across planning periods. These are treated as the invariant variables \( (D) \) for the multi-period problem. It is assumed that having identified uncertainty perfectly, it will be possible to implement the specific input operating policy that can improve the current period the most.

Robust Correction: With multi-period correction, robust implementation translates to requiring the correction profile parameters at each collocation point and processing times to be identical across each
member of the set of uncertain operations for a product stage pair. This corresponds to the robust correction case (MP2).

\[
\max_{s_p, u_p, v_p} \sum_p w_p \psi_p \\
\text{s.t.} \quad f_{tp}(z_p, u_p, v_p; \theta_p^p) = 0 \\
\quad u_p(t) = \hat{u}(t) + K^T(t) \delta z_p(t) \\
\quad V_p, K^T(t), t_{oi} \in \mathcal{D} \quad (MP2)
\]

Here, robust gain parameters are treated as invariant design variables, and the state and input profile parameters as periodic variables.

Robust Input: Another option is to solve the problem (PI) with a robust input policy for all uncertain operations. This is achieved by treating profile parameters at any collocation point as invariant across periods and the processing times to be equal across the uncertain operations, resulting in problem (MP3).

\[
\max_{s_p, u_p, v_p} \sum_p w_p \psi_p \\
\text{s.t.} \quad h_{tp}(z_p, u_p; \theta_p^p) = 0 \\
\quad V_j, u_j(t), t_0 \in \mathcal{D} \quad (MP3)
\]

For the three cases considered the following property holds.

**Property 1:** For problems MPl, MP2 and MP3, \(<f>_\text{MPl} > <f>_{\text{MP2}} > <f>_\text{MP3}\) is satisfied, where \(<f>\) are the objective function values.

**Proof:** The robust input case (MP3) is the most constrained of all. It corresponds to the Robust Correction case (MP2) with \(K^T = 0\). In this case the reference input policy will turn out to be the robust input policy. Also, the solution of (MP3) is feasible for (MP1) and can be obtained by adding an extra robustness constraint to the perfect information case (MPl). Similarly, the solution of (MP2) is feasible for (MPl) as it can be obtained by adding additional correction and robust gain constraints to the perfect information model (MP1). Based on this argument, the objectives of these formulations will follow the above relation.

The Perfect Information and Robust Input scenarios correspond to the "Wait and See" and "Here and Now" situations for planning under uncertainty respectively. The performance difference between these is known as the Expected Value of Perfect Information (EVPI) [11]. The Robust Correction approach will be able to recover some of this potential, without perfect information, while providing the same implementation advantage as the Here and Now case.
3.3 Constraints on the Input

So far, the formulation is developed for unconstrained input policies. A real situation may require addressing upper and lower bounds on the input policies for reasons of safety and operability. The issue of correction in the face of an active input constraint requires some modification. In this situation, the input policy would be to follow the active bound without any need for correction. If robust correction is still imposed, it could lead to a compromise in the performance of other periods or violation of the input constraint in the active period. To avoid this, correction must be dropped for the period corresponding to a constraint activity. This is similar to an over-ride of the correction strategy for regions of constraint activity by a policy to simply follow the active constraint.

The over-ride situation requires switching between a corrected policy and a bound, which is a discrete decision. To incorporate these in the overall formulation, a continuous switching parameter \( A \) is used that takes discrete values in different regions with the following formulation. Consider an upper bound \( u^u \) on the input profiles and \( u^c \) the result of the robust corrected input profile.

\[
S(t) = u^c(t) - u^u \\
A(t) \cdot \delta(t) \geq 0 \\
X(t) \cdot S(t) \geq \delta(t) \\
0 \leq X(t) \leq 1
\]

A similar formulation for valve switching is used by Gopal and Biegler [7]. With these constraints, the switching parameter takes a value one when \( S \) is positive and a value zero when \( S \) is negative. The expression for the implemented profile \( u_o \) (\( o \in Oij, i \in I, j \in J \)) uses this information to achieve the desired switching between the corrected policy and the operating bound in the following manner.

\[
u_o(t) = (1 - \lambda_o(t)) \cdot [u^c] + \lambda_o(t) \cdot [u^U]
\]

This insures that the input profile remains within bounds. These constraints are discretized and imposed at each collocation point.

3.4 Overall Formulation

We extend the processing and planning formulation in Bhatia and Biegler[1] to address the overall problem as follows. For simplicity, consider the case with uncertainty in one product stage operation only. We will generalize this for other cases later.

Consider the index \( o \) for dynamic process models of an uncertain operation, resulting from possible combinations of uncertain parameter instances therein. The set \( Oij \) includes all \( o \) dynamic process models corresponding to processing product \( i \) in stage \( j \). For uncertainty in a single product stage operation, each combination of uncertain parameters corresponds to a scenario or period \( p \) in the planning problem, where \( p = 1, ...iV> \). In addition dynamic process models for deterministic operations are also included. If product \( i = I \) in stage \( j = J \) is the only uncertain operation, then the set \( O_o \) includes all process models \( o \) corresponding to the instances of uncertain model parameters. The multiperiod planning formulation corresponding to this situation, in the presence of an upper bound on the input profile, for the perfect information case is of the form (PI).
\[
\begin{align*}
\text{max}_{i,\eta,\nu} & \quad \sum_p w_p \psi_p (CT_{pj}, V_j, Q_{pi}) \\
\text{s.t.} & \\
& h_{\psi ij}(x, u, v) = 0 \quad \forall \alpha \in O_{ij}, i = T, j = J \quad \text{Closed loop process models} \\
& z^L \leq z \leq z^U \\
& \delta_{ij}(t_{lm}) = u_{ij}(t_{lm}) - u^U \quad \forall \alpha \in O_{ij}, i = T, j = J, /, m \\
& \lambda_{ij}(t_{lm}) \cdot \delta_{ij}(t_{lm}) \geq 0 \quad \forall \alpha \in O_{ij}, i = T, j = J, /, m \\
& \lambda_{ij}(t_{lm}) - \delta_{ij}(t_{lm}) \geq \delta_{ij}(t_{lm}) \quad \forall \alpha \in O_{ij}, i = T, j = J, /, m \\
& 0 \leq \delta_{ij}(t_{lm}) \leq 1 \\
& U_{ij}(U_m) = (1 - \delta_{ij}(U_m)) \cdot [u_{ij}(t_{lm})] + \lambda_{ij}(t_{lm}) \cdot [u^U] \quad \forall \alpha \in O_{ij}, i = T, j = J, /, m \\
& \text{Switching} \\
& z^0_{pij} = f(z^0_{pij}) \quad \forall p, i, j, j' \neq 1, j' = j - 1 \\
& z^0_{pij} = z^0_{pi} \quad o = p, o \in O_{ij}, i = T, j = J \\
& t_{pij} = t_{pi} \quad o = p, o \in O_{ij}, i = T, j = J \\
& Z^0_{pij} = 0 \quad \forall j \neq 0 \\
& U_{pij} = S_{pij} \quad \forall j \neq 0 \\
& B_{pij} = f(z^f_{pij}) \quad \forall p, i, j = N_{ji} \\
& V_j \geq S_{ji} B_{pij} \quad \forall p, i, j \in J_d \\
& S_{ji} B_{pij} \geq 0 \quad \forall p, i, j \in J_d \\
& N_{pij} = \frac{S_{pij} B_{pij}}{S_{pi}} \quad \forall p, i \\
& \sum_{k=1}^{N_p} \sum_{i=1}^{N_{pi}} NPRS_{pi} = n_{pi} \quad \forall p, i \\
& \sum_{k=1}^{N_p} NPRS_{pik} = n_{pik} \quad \forall p, k \\
& NPRS_{p} \leq n_{pi} - 1 \quad \forall p, i \\
& CT_{pj} = Z & i \left( n_{pi} t_{pij} + \sum_{k=1}^{N_p} SL_{pik} j NPRS_{pik} \right) \quad \forall p, j \\
& CT_{pj} \leq H \quad \forall p, j \\
& SL_{pik, j} + t_{pik, j} = t_{pik, j+1} + SL_{pik, j+1} \quad \forall p, i, j, j' < J \\
& V_j \geq 0, n_{pi}, B_{pi} \geq 0, NPRS_{pik, j} \geq 0, SL_{pik, j} \geq 0 \\
\end{align*}
\]

In (PI), index \( p \) is for a period in the multi-period problem and \( h^{c} \) are closed loop process models as in (MP2). Variables \( Z_{ij}(t_{lm}) \) and \( T_{Xij}(t_{lm}) \) are coefficients in polynomial approximations to the profiles at discretized points \( U_m \) in time for product \( i \) in stage \( j \). A weighted profit objective is maximized, that is a function of stage cycle times \( (CT_{pj}) \), equipment sizes \( (V^n) \) and production \( (Q_{pi}) \) in each period. The closed loop dynamic models are included via the functions \( h^{c} \) (discretized differential algebraic system of equations) for the uncertain operation.

To distinguish between dynamic stages that involve uncertainty, consider the set \( J_u \) as a subset of \( J^{<0} \). Similarly, let the set \( I_u(J_u) \) contain all products \( i \) that contribute to the uncertain operations for the stages \( j \in J_u \). Stages that are not modeled dynamically are treated as recipe based in the formulation (MI), as operations with fixed processing time. These stages \((j & Jd)\), might also respond to the uncertainty in other units by adjusting the processing time or recipe. We do not consider this possibility although it could also be handled in the multiperiod formulation. Recipe based processes offer no dynamic processing freedom and are treated as fixed time operations for all planning periods.
4 Example 1 - Single Dynamic Stage

The above formulation is used to solve the three stage problem in [1], now with uncertainty in the processing parameters of one product.

![Diagram showing the process](image)

Figure 2: Example 1: Three stage example with dynamic reactor.

This example involves a dynamic reactor and two recipe based blenders (Figure 2). The reactor supports a competing reaction, where B is the desired product. Three similar products are processed in this plant, using an identical sequence of stages. Each reactor stage operation involves two kinetic reaction parameters ($\theta_i$ and $\theta_i^t$).

4.1 Single Product Uncertainty

First, consider uncertainty in the reactor operation for just one product ($i = 1$). Here, the subset of stages that are modeled dynamically is $J^\circ = \{1\}$ corresponding to the reactor. Further, the subset of stages with uncertain operations is $J_u = \{1\}$. The set of products that have uncertainty in their operation in the members of $J_u$ belong to the set $I_u(j)$ and for this situation $I_u(1) = \{1\}$, as only the first product has uncertain processing in the dynamic reactor. For product 1, two reaction parameters $\theta_i$ and $\theta_i^t$ are considered uncertain, with 5 and 3 instances each. Only ten of the fifteen possible operations for product one are considered likely. These ten operation models ($\alpha = 1, \ldots, 10$) for the first product in the dynamic reactor are included, along with a nominal model for correction purposes ($\alpha = 11$), and deterministic models for the second and third products ($\alpha = 12$ and 13). Using the ten likely reactor operations for the first product along with the operations for the other products leads to ten planning scenarios for the multiperiod problem.

For this situation, parameter variations accounted for $\alpha_i$ and $\beta_i$ parameters correspond to the values shown in Table 1.

<table>
<thead>
<tr>
<th>Operation</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_i$</td>
<td>2.2</td>
<td>2.2</td>
<td>2.0</td>
<td>2.2</td>
<td>1.8</td>
<td>1.8</td>
<td>1.8</td>
</tr>
<tr>
<td>$\beta_i^t$</td>
<td>0.46</td>
<td>0.47</td>
<td>0.50</td>
<td>0.53</td>
<td>0.55</td>
<td>0.46</td>
<td>0.47</td>
</tr>
<tr>
<td>Operation</td>
<td>8</td>
<td>9</td>
<td>10</td>
<td>11</td>
<td>12</td>
<td>13</td>
<td>-</td>
</tr>
<tr>
<td>$\alpha_r$</td>
<td>1.8</td>
<td>1.8</td>
<td>1.8</td>
<td>1.98</td>
<td>2.0</td>
<td>3.0</td>
<td>-</td>
</tr>
<tr>
<td>$\beta_i$</td>
<td>0.50</td>
<td>0.53</td>
<td>0.55</td>
<td>0.502</td>
<td>0.4</td>
<td>0.5</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 1: Parameter values for different periods.
Solution Strategy

To solve the overall multi-period planning problem with uncertainty in the processing parameters, a strategy for good initializations is adopted. These are obtained by solving individual aspects of the problem until the entire problem is properly initialized.

First, each of the individual reactor operations are optimized separately by solving problems (RO) for each reactor operation, where the desired product is maximized in a fixed time of 0.6 hours.

\[
\begin{align*}
\max & \quad x^f \\
\text{s.t.} & \quad h_{ooij}(z_{ooij}, u_{ooij}) = 0 \\
& \quad t_{ooij} = 0.6 \quad (RO)
\end{align*}
\]

The reactor operations corresponding to the first product are then combined in a multi-period corrected reactor problem, where the objective is to maximize the expected conversion to the desired product, subject to robustness constraints on the correction gains and the duration of each operation. This problem (MRO) is initialized with the solutions of the individual reactor problems (RO).

\[
\begin{align*}
\max & \quad \sum_{a=1}^{10} w_a x_{a,f} \\
\text{s.t.} & \quad h'_{ooij}(z_{ooij}, u_{ooij}, K_{ooij}) = 0 \\
& \quad K_{ooij}(t_{im}) = K_{i1f}(t_{im}) \forall q \\
& \quad t_{ooij} = 0.6 \quad (MRO)
\end{align*}
\]

Next, the individual planning problems are optimized using the initializations from the previous step. These provide initialization for the multi-period planning problems at the next step. The perfect case (PI) is solved first. This is followed by a series of robust correction cases, wherein the robust gains are relaxed from best constant to piecewise constant to best time varying values (RC). From this, the robust input model is solved (RI).

Results and Discussion

The results for the individual reactor operation problems (RO) are summarized in Table 2. Also shown are the corresponding values \(x^\wedge\) for the operations of product one corresponding to the corrected multi-period reactor problem (MRO). Highest conversion is achieved in the perfect information individual problems. With robust correction, periods with smaller variation in the parameters perform closer to the corresponding perfect information cases.

Three planning problems, consistent with the ones in Bhatia and Biegler [1] were solved for the following scenarios. Problem PI involves minimizing an operating cost, proportional to stage cycle times, for meeting specified production requirements of each product within an existing facility. Problem P2 involves maximizing revenues from operating a given facility for a specified planning horizon. Problem P3 maximizes an overall profit objective that is a function of fixed design costs, revenues and operating costs. In this example we considered both ZW and UIS transfer policies.

The results for individual periods in the planning Problem PI appear in Table 3, for each of the perfect (PI), robust corrected (RC) and robust input models (RI).
Table 2: Results for reactor subproblems Rl-13 and MRO.

<table>
<thead>
<tr>
<th>Operation</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X_f )</td>
<td>0.493</td>
<td>0.489</td>
<td>0.498</td>
<td>0.473</td>
<td>0.467</td>
<td>0.533</td>
<td>0.529</td>
</tr>
<tr>
<td></td>
<td>0.484</td>
<td>0.485</td>
<td>0.496</td>
<td>0.470</td>
<td>0.463</td>
<td>0.529</td>
<td>0.527</td>
</tr>
<tr>
<td>Operation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( x_{af} )</td>
<td>0.519</td>
<td>0.509</td>
<td>0.503</td>
<td>0.532</td>
<td>0.442</td>
<td>0.449</td>
<td></td>
</tr>
<tr>
<td>( x_{bf} )</td>
<td>0.518</td>
<td>0.508</td>
<td>0.501</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 3: Periodic operating costs ($) for problem PI (small uncertainty).

The operating cost for each period with robust correction is close to the corresponding cost for the perfect information case. Also, this is a significant improvement over the robust input case while offering a similar implementation advantage. The results for the weighted objective function, that reflects expected performance, for all planning scenarios considered are presented in Table 4.

<table>
<thead>
<tr>
<th>Policy</th>
<th>Problem</th>
<th>PI</th>
<th>RC</th>
<th>RI</th>
<th>EVPI ($)</th>
<th>% recovered</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZW</td>
<td>Min.0p1</td>
<td>24,761.11</td>
<td>24,762.24</td>
<td>24,822.31</td>
<td>61.20</td>
<td>98.2</td>
</tr>
<tr>
<td></td>
<td>Max.(^p)</td>
<td>48,992.61</td>
<td>48,990.59</td>
<td>48,883.15</td>
<td>109.46</td>
<td>98.2</td>
</tr>
<tr>
<td></td>
<td>Max.(*p)</td>
<td>28,251.28</td>
<td>28,248.70</td>
<td>28,108.59</td>
<td>142.69</td>
<td>98.2</td>
</tr>
<tr>
<td>UIS</td>
<td>Min.(^\pi)</td>
<td>21,692.01</td>
<td>21,720.61</td>
<td>21,797.05</td>
<td>105.03</td>
<td>72.8</td>
</tr>
<tr>
<td></td>
<td>Max.0P2</td>
<td>49,525.63</td>
<td>49,488.21</td>
<td>49,364.26</td>
<td>161.37</td>
<td>76.8</td>
</tr>
<tr>
<td></td>
<td>Max.0p3</td>
<td>34,055.09</td>
<td>33,989.83</td>
<td>33,825.78</td>
<td>216.10</td>
<td>70.6</td>
</tr>
</tbody>
</table>

Table 4: Weighted objectives ($) for problems P1,P2 and P3.

The EVPI reported is the difference between the performance of the perfect information case and the robust input case.

\[
EVPI = \phi(PI) - \phi(RI)
\]

\[
\%recovered = \frac{\left|\phi(RC) - \phi(RI)\right|}{EVPI} \times 100\%
\]

This reflects the potential for improvement that exists. A part of this potential can be recovered or realized by the robust correction approach.

The potential improvement suggested for the ZW policy is lower than UIS, as it is in some sense limited by the requirement of Zero Wait for a batch between stages. For a similar reason, almost all of this potential
is realizable. For all problems (PI, P2 and P3) with the ZW policy, close to 98% of the EVPI is closed with robust correction. The value of EVPI is largest for the profit maximization problem (P3), which involves more planning decisions than any other problem.

For ZW problems, all reactor operations have an equal duration of 0.6 hours. A further reduction in time provides no incentive as the third stage (a blender) becomes the bottleneck stage. For all problems PI, P2 and P3 the final conversions and hence the batch sizes for the uncertain product operation in each period are almost the same for the PI and RC cases, differing in only two cases (largest uncertainty) by a mere 0.2%. In all these problems, for a fixed reaction time, achieving a higher conversion contributes to improving the objective. For the robust input case, all periods reflect a lower desired conversion than in the perfect information case, as low as 1.5%.

The UIS problems, being more relaxed than the ZW problems, are characterized by a larger EVPI for all scenarios. Here, any improvement in a stage operation in terms of higher conversion or reduced duration directly leads to lower operating costs or higher revenues. In the ZW case, this effect is masked to some extent by the presence of idle time in the schedule. The improvements in each period with robust correction, though aided by the assumption of unlimited storage at zero cost, are still unable to close as high a portion of EVPI present in the UIS problems.

In the UIS problems, PI case has reactor operations of different durations to improve the weighted objectives. All operations in the RC and RI cases are forced to have equal duration, the RI input operations last 2.5% longer with no clear trend for improvement in the reaction conversions.

Constrained Input

The problems were solved with an upper bound of 5.0 imposed on the transformed temperature profile for each reactor operation. The switching formulation successfully handled the upper bound. In no period for any problem was the constraint violated. Further, for periods where the upper bound on the input policy became active, the switching function took appropriate values.

<table>
<thead>
<tr>
<th>Policy</th>
<th>Problem</th>
<th>PI</th>
<th>RC</th>
<th>RI</th>
<th>EVPI ($)</th>
<th>% recovered</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZW</td>
<td>Min. $^p$</td>
<td>24,891.98</td>
<td>24,896.74</td>
<td>24,917.32</td>
<td>25.34</td>
<td>81.0</td>
</tr>
<tr>
<td></td>
<td>Max. $^p$</td>
<td>48,758.56</td>
<td>48,749.38</td>
<td>48,713.24</td>
<td>45.32</td>
<td>79.7</td>
</tr>
<tr>
<td></td>
<td>Max. $^d$</td>
<td>27,946.18</td>
<td>27,935.48</td>
<td>27,887.09</td>
<td>59.09</td>
<td>81.9</td>
</tr>
<tr>
<td>UIS</td>
<td>Min. $^d$</td>
<td>21,949.34</td>
<td>21,975.32</td>
<td>22,022.07</td>
<td>72.73</td>
<td>64.3</td>
</tr>
<tr>
<td></td>
<td>Max. $^p$</td>
<td>49,171.41</td>
<td>49,133.87</td>
<td>49,076.81</td>
<td>94.60</td>
<td>60.7</td>
</tr>
<tr>
<td></td>
<td>Max. $^d$</td>
<td>33,548.78</td>
<td>33,491.36</td>
<td>33,402.70</td>
<td>146.08</td>
<td>60.7</td>
</tr>
</tbody>
</table>

Table 5: Weighted objectives for single product uncertainty and constrained input

The constraints on the input lead to a deterioration in the weighted objective functions for each planning problem. The EVPI for the planning problems are now smaller, 41% of the EVPI in the corresponding unconstrained problems for ZW and correspondingly about 65% for UIS. The recovery of EVPI with robust correction is about 80% for all ZW problems and close to 60% for the UIS problems. These figure are lower than the corresponding figures for an unconstrained policy. Although the correction is somewhat specific to each policy, in view of the over-ride option, the effect of the input constraint is to partially reduce the recovery of EVPI in the constrained case.

Although the EVPI figures are not large compared to the weighted objective function values of the
corresponding problems, the trends for closure with the proposed approach are encouraging. Also, so far uncertainty is considered only in one product. Next, uncertainty is extended to reactor operations for other products and the approach is further analyzed.

### 4.2 Multiple Product Uncertainty

Uncertain operations can exist in all operations $ij$, involving a product $i$ and stage $j$. For any uncertain operation $ij$, combinations of the instances of individual parameters give rise to a number of possible operations that need to be included. Further, each one of these stage-product operations combine to generate possible planning scenarios, or periods in the multi-period planning problem. A general representation for this purpose is explained through Figure 3.

![Dynamic Process Models](image)

**Figure 3: Representation with multiple uncertain operations.**

The planes on the top of the figure represent $P$ planning scenarios, where products are processed in the same sequence in $N_j$ stages. The large circles in the bottom of the figure correspond to a product stage operation and contain all probable operations that arise from the instances of uncertain parameters within each product stage pair. The only processing information required while planning involves stage processing times, that affect production span, and final batch states, that affect number of product batches or production capacity.

A dynamic process model is included for every probable combination of uncertain parameter instances, for each product stage operation. In order to avoid duplication of process models in each planning scenario, processing information is picked up from the relevant operation models through a mapping $Af_j(O)$ which maps an operation for product $t$ in stage $j$ in the planning scenario $p$, keeping the size of the model from growing too large. This also implies that any instance of a product stage operation will be processed identically, irrespective of the planning scenario it appears in.

In this example, the reactor is the only dynamic stage ($J_d = \{1\}$), uncertainty is extended in the reactor operations ($J_u = \{1\}$) for all three products, so $I_u(1) = \{1,2,3\}$. One uncertain reaction parameter is considered with two instances for each of the three products. After including the two uncertain operations
(1 and 2 for the first product, 3 and 4 for the second product and 5 and 6 for the third product) and a reference reactor operation model for each product, the total number of reactor models in the problem is nine. Both parameter instances are likely and the number of operations that contribute to planning periods are thus two for each product. Each of these combine to give eight planning periods. The map $A'(o)$ for this situation corresponds to $A_v^1 = 1, A_v^2 = 3, A_v^3 = 5; A_v^1 = 2, A_v^3 = 3, 4, 5$ and so on up to $A_v^2 = 2, A_v^3 = 4, A_v^3 = 6$. The table of uncertain parameter values for all periods, are shown in table 6.

<table>
<thead>
<tr>
<th>Operation</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_v$</td>
<td>1.8</td>
<td>2.2</td>
<td>1.8</td>
<td>2.2</td>
<td>2.8</td>
<td>3.2</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>$\theta_l$</td>
<td>0.5</td>
<td>0.5</td>
<td>0.4</td>
<td>0.4</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.4</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 6: Parameter values for multiple product uncertainty.

Solution Strategy

The initialization scheme used to solve this case was similar to the one previously used for the case with uncertainty in a single product operation. All individual operations were first solved separately to maximize desired conversion in a fixed time. These were used to initialize solution of the multiperiod reactor problems, this time one for each product. The individual planning problems were then resolved from the previous solutions leading up to the multiperiod planning problems.

Results and Discussion

The performance of the individual reactor subproblems are shown in Table 7. With robust correction, the performance of the periods are close to perfect for each product.

<table>
<thead>
<tr>
<th>Operation</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x^{2}_{R}$</td>
<td>0.519</td>
<td>0.481</td>
<td>0.557</td>
<td>0.512</td>
<td>0.449</td>
<td>0.436</td>
</tr>
<tr>
<td>$x^{2}_{R}$</td>
<td>0.519</td>
<td>0.481</td>
<td>0.556</td>
<td>0.512</td>
<td>0.448</td>
<td>0.436</td>
</tr>
</tbody>
</table>

Table 7: Results for reactor operations $R_1 - R_6$.

The results for the weighted objectives of problems P1, P2 and P3 are shown in Table 8. The EVPI values in all the problems for both ZW and UIS policy are about twice as large, compared to the single product uncertainty case with ten periods. The trends for closure are similar. For ZW problems, about 98% of EVPI is recovered at least and up to 99.6% for problem P3. For UIS the closure is up to 69% for problems P1 and P3 and 87% for problem P2.

For the ZW policy, as before, the periods for each product in the RC case reflect a conversion extremely close to those in the PI case. For the RI cases, the conversions are slightly different (up to 1.2% for product 1, 1.4% for product 2 and 0.2% for product 3). This is true for all problems PI and P2. For problem P3, the third product reflects a larger deterioration in one of its periods of 0.9%.

For the UIS policy, no clear trend is observed. The reactor operations in the RC and RI cases respond with less efficient net production of the desired product. These occur due to larger durations to achieve
Table 8: Weighted objectives for P1,P2 and P3 with multiproduct uncertainty.

even a higher conversion or a lower conversion achieved in a lower time or due to both. The duration of operations for each product in the RI case are larger than those of the RC case.

It is observed that the values for EVPI, are now larger with the uncertainty present in all products. For improvement of the overall profit objective in problem P3, EVPI as a percentage of the overall objective function is 1.46% for UIS and 1.1% for ZW policies for this problem.

**Constrained Input**

An upper bound was imposed on the reactor input profiles as before. The weighted objectives for each planning problem with uncertainty in all products and an input constraint are shown in Table 9. As before, the presence of the input constraint lead to a smaller value of EVPI for all problems. The trends for EVPI recovery are however similar to those observed in the unconstrained case. For ZW the recovery is almost complete.

Table 9: Weighted objectives for uncertainty in all products with constrained input

A complicating aspect that has not been addressed here so far is one of implementation of the scheduling decisions or the plan for different periods. In a scenario where any period is equally likely and it is not known beforehand which period will turn up next, for instance if different qualities of feed are available for use it would be hard to decide on a plan for the production. Iyer and Grossmann [12] consider operational decisions including startup and shutdown of units in different planning periods for utility systems with piecewise constant demand variations. They address the multiperiod problem through a decomposition approach but for known variation of demands in planning periods.

Consider the situation where uncertainty comes across different production cycles, but does not vary within each cycle. In this situation, implementing any robust policy, either robust input or robust correction, and comparing the observed state profiles with those available in each period, would help identify $\theta_p$ for each product, implying perfect information. Subsequently, the solution of the perfect information period
corresponding to the identified \( \theta_p \) could be implemented and performance close to optimal could be achieved. The only EVPI loss would be dictated by the part of the production cycle dedicated to identifying the period.

The proposed approach is more relevant in the case where the periods for each uncertain operation change within a production cycle. In such a scenario, the production plan would require implementation with some checks required. For instance, in problem P2, the production plan would use robust correction to process all products until the minimum requirements for all are met. The remaining part could be dedicated to making the more expensive product. The UIS policy is sequence independent and the products could be processed in any order. For the ZW, policy it turns out that for this problem, all products required processing for an equal duration in each stage. This renders the ZW case to be sequence independent too.

For the more general ZW case, where all products are not identical in their time requirements at all stages and the problem is sequence dependent, the robust duration constraints still ensure each period of any operation has the same processing time. In this case, the number of product batches would be different in each period.

For this one dynamic stage example the recovery of EVPI is significant, although the EVPI is small compared to the benefits of integrating dynamic processing and planning decisions. To extend the analysis to more than one uncertain stage we consider the two stage example in Bhatia and Biegler [1].

### 5 Example 2 - Two Dynamic Stages

The second example is the four stage example from Bhatia and Biegler [1]. It involves two dynamic stages, a reactor that benefits from a dynamic temperature profile and a batch distillation column that allows a dynamic reflux ratio profile. Column dynamics are included using the shortcut batch distillation model without holdup in Logsdon et al. [13] and involves equilibrium relations, Gilliland’s correlation and Underwood’s equations apart from the residual collocation equations. Here we will consider the overall profit maximization problem (P3) for both the constrained and unconstrained input cases.

Processing for all products is identical in the reactor, where a binary feed is processed to give a six component mixture via a mechanism involving three reversible reactions. The next two recipe based stages cool the batches and remove one waste component. The feed to the final column stage is treated as a binary mixture of the desired component and other lumped components. In the column, products of different purity are separated.

Uncertainty is considered now in both dynamic stages. The situation considers two sets of feed that have to be accommodated. These give a difference in one reaction parameter for the reactor operations. The final condition of the batch after the reactor, from the two feeds, will thus be different. We assume that recipes that involve cooling and waste separation in the second and third stage do not require any modification. The initial binary composition for the column operations could be identical for the two feeds, as both of the five component mixtures at the end of the third stage could result in identical binary compositions. The column feed is one uncertain parameter. Additionally, the different batches are considered with two different values for relative volatility.

The uncertainty representation for this situation involves two dynamic stages, both uncertain and hence \( J_d = J_u = \{1,4\} \). All product operations in both stages are uncertain, hence \( \mathcal{I}_u(1) = \mathcal{I}_u(4) = \{1,2,3\} \). There is one uncertain parameter for the reactor operations with two instances arising from the difference in feed. This gives two different feeds for the column operations of all products. In addition, relative volatility in the column parameter is considered uncertain with two instances. Each product operation differs in the
purity specification imposed. Consequently, the total number of scenarios for the planning problem are four, arising from the two reactor and two column operations. There is no need to include separate reactor models for each product, although including the nominal column operation for each product requires a total of five operations for each product and fifteen operations in all.

**Solution Strategy**

The solution strategy was similar to the one used for solving the first example, relying on subproblems that provide good initializations to larger aspects leading up to the final overall formulation. This example was solved with an upper bound constraint imposed on both the input policies, the temperature in the reactor and the reflux ratio profile in the distillation column.

**Results and Discussion**

The weighted planning objectives for the profit maximization problem for ZW policy are presented in Table 10. It is observed that EVPI for the planning problems in this example are considerably larger.

<table>
<thead>
<tr>
<th>(Unconst.)</th>
<th>PI</th>
<th>RC</th>
<th>RI</th>
<th>EVPI ($)</th>
<th>% recovered</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi = \sum w_i \phi_i$</td>
<td>18,517.59</td>
<td>18,358.74</td>
<td>16,996.85</td>
<td>1,520.74</td>
<td>89.4</td>
</tr>
<tr>
<td>01</td>
<td>17,551.35</td>
<td>17,532.45</td>
<td>16,996.85</td>
<td>554.50</td>
<td>96.6</td>
</tr>
<tr>
<td>02</td>
<td>20,054.70</td>
<td>19,737.05</td>
<td>16,996.85</td>
<td>3,057.85</td>
<td>89.6</td>
</tr>
<tr>
<td>03</td>
<td>16,996.85</td>
<td>16,840.12</td>
<td>16,996.85</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>04</td>
<td>19,467.46</td>
<td>19,308.12</td>
<td>16,996.85</td>
<td>2,470.61</td>
<td>93.6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(Const.)</th>
<th>PI</th>
<th>RC</th>
<th>RI</th>
<th>EVPI ($)</th>
<th>% recovered</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi = \sum w_i \phi_i$</td>
<td>18,448.35</td>
<td>17,999.82</td>
<td>16,996.47</td>
<td>1,513.88</td>
<td>70.4</td>
</tr>
<tr>
<td>01</td>
<td>17,479.23</td>
<td>17,431.96</td>
<td>16,934.47</td>
<td>544.76</td>
<td>91.3</td>
</tr>
<tr>
<td>02</td>
<td>19,978.33</td>
<td>19,767.31</td>
<td>16,934.47</td>
<td>3,043.86</td>
<td>93.1</td>
</tr>
<tr>
<td>03</td>
<td>16,934.47</td>
<td>16,181.46</td>
<td>16,934.47</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>04</td>
<td>19,401.39</td>
<td>18,618.91</td>
<td>16,934.47</td>
<td>2,466.92</td>
<td>68.3</td>
</tr>
</tbody>
</table>

Table 10: Example 2, weighted and individual objectives in each period for uncertainty in all products, constrained and unconstrained.

For the unconstrained case, the EVPI is 8.2% of the weighted profit objective of the perfect information case. This is larger than the 7% incentive in simultaneously incorporating dynamic processing and planning decisions for this example. The EVPI recovery for this case with the proposed approach is 89% ($1,358). For two dynamic stages with uncertainty, the proposed approach is able to recover a considerable portion of a more significant EVPI. For the constrained case, EVPI is only slightly smaller but the recovery with the proposed approach is smaller as well.

This example reflects that the effect of uncertainty, in terms of the performance gap between the perfect information and the robust input case, becomes more pronounced with the number of uncertain stage operations as compared to the number of uncertain products. For Example 2, this is of the same order as the savings that were realized in integrating processing decisions in planning in the first place. The proposed (RC) approach is promising, in that it is able to realize most of the predicted gap while providing the same implementation advantage as with the robust input case. This practical approach helps realize the true potential of processing decisions in planning.
Computational results

All problems in this work were solved using the NLP solver CONOPT through the GAMS modeling system [4]. Typical problem size and solution time data are reported in Table 1.

<table>
<thead>
<tr>
<th>Model</th>
<th>Equations</th>
<th>Variables</th>
<th>CPU time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PI</td>
<td>3294</td>
<td>3091</td>
<td>5.6</td>
</tr>
<tr>
<td>RC</td>
<td>3646</td>
<td>3223</td>
<td>6.7</td>
</tr>
<tr>
<td>RI</td>
<td>3594</td>
<td>3091</td>
<td>6.3</td>
</tr>
</tbody>
</table>

Table 1: Example 2, Problem size and CPU times

The reported CPU times are for an HP9000 work station but it must be noted that the problems were solved using good initializations, through sequential solution of the PI, RC and RI cases.

6 Future Work

The overall problems, relying on a multiperiod formulation are of very large size. The computational time requirements of all problems are reported. The main drawback in being able to implement the proposed approach lies in the explosive size of multiperiod problems for a realistic number of periods. If uncertainty in planning parameters is also allowed to contribute scenarios, then planning periods as well as dynamic process models would lead to a large problem. The future work will thus address computational aspects of the overall multiperiod problem. Decomposition strategies tailored for the proposed approach will be developed.

Acknowledgments

Financial support from the Department of Energy under Grant No. DE-FG02-85ER13396 is gratefully acknowledged for this work.

References


