Integration of Scheduling and Control Under Stochastic Parametric Uncertainty with Varying Unit Operation Times for Chemical Batch Plants: A Back-Off Approach

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Abstract: A new back-off methodology is presented in this work as an approach for solving MIDO formulations arising for the optimal scheduling and control of flow-shop batch plants under stochastic parametric uncertainty. The proposed algorithm decomposes the MIDO problem into a scheduling problem, a dynamic optimization problem and a unit time operation minimization problem. These problems are solved iteratively using back-off terms. Parametric uncertainty is modeled using statistical distribution functions and are embedded in the algorithm to ensure dynamic feasibility of the optimal control actions under stochastic realizations in those parameters. The proposed algorithm identifies scheduling and control decisions offline. To exemplify this methodology, the integration of scheduling and control of a flow-shop batch plant is considered. The results show that unit operation times chosen from optimization are better suited to accommodate stochastic parametric uncertainty while the control actions enforce process operational and product quality constraints at reasonable costs.

Keywords: Flow-Shop Batch Plants, Optimal control, Uncertainty, Back-Off Approach, Stochastic Modelling.

1. INTRODUCTION

Traditionally, chemical processes are modeled and optimized as non-interactive problems for each of the decision layers, which often assume perfect (ideal) conditions of operation. While yielding economically attractive solutions for each decision layer, these solutions face multiple complications when implemented in real systems due to information mismatch, thus leading to suboptimal or infeasible solutions. To address this issue, methodologies for the integration of different decision layers have been reported (Dias and Ierapetritou, 2017; Pistikopoulos and Diangelakis, 2016; Rafiei and Ricardez-Sandoval, 2020). Those methods have shown to improve the performance of the studied systems with varying levels of success (Baldea and Harjunkoski, 2014; Engell and Harjunkoski, 2012; Koller and Ricardez-Sandoval, 2017). However, simultaneous approaches are often set to solve complex Mixed-Integer Dynamic Optimization (MIDO) problems, which, after discretization, become large-scale Mixed-Integer Non-Linear Programming (MINLP) problems that may become computationally intractable due to model inflation and complexity.

While scheduling aims to determine product sequences and production parameters for profit maximization, process control strategies aim to ensure the achievement of production goals during operation. A few approaches for integration of scheduling and control had already been proposed (Beal et al., 2018; Koller et al., 2018; Zhuge and Ierapetritou, 2012). Typically, uncertainty in optimal scheduling and control is omitted or simplified by deterministic assumptions made in the modelling part to ease the computational efforts. Studies implementing stochastic parametric uncertainty has been conducted using a two-stage stochastic programming approach (Chu and You, 2013) and, within our research group, an earlier version of a back-off methodology (Valdez-Navarro and Ricardez-Sandoval, 2019). In the back-off approach, the key idea is to move away from a highly attractive economic (though infeasible) solution to another point that is still economically competitive but has the capacity to remain dynamically feasible under stochastic realizations in the uncertain parameters. The back-off methodology has been successfully implemented for the integration of design, scheduling and control under uncertainty for multi-product units (Koller et al., 2018) and for the integration of scheduling and control of a batch process (Valdez-Navarro and Ricardez-Sandoval, 2019). In those previous back-off studies, processing times for each unit remained fixed, which may limit plant performance under uncertainty.

In the present work a novel implementation for back-off terms is presented. The key novelty is the consideration of varying unit operation times directly affected by the back-off terms. Additionally, to better reflect the effect of the varying unit operations times in the scheduling problem, a continuous-time formulation is considered. Hence, a more economically attractive operation regime can be found by the formulation presented in this work. A case study featuring a flow-shop batch plant will be used to exemplify the benefits of the proposed decomposition framework.

2. PROBLEM STATEMENT

Consider a chemical flow-shop multi-unit multi-product batch plant composed of N_{Pr} set of processes, N_E set of equipment, and N_R set of recipes. A chemical process is described by N_p mechanistic dynamic models (f_p), N_q inequality constraints (h_q) and N_r equality constraints (k_r), which may include safety and operational constraints, affected by a set of parameters Ψ composed by deterministic parameters (ψ_{Nom}) and random parameters (ψ_{Unc}) characterized by probability distribution functions. The set C has size N_C and holds the cost information of raw materials, waste by-products and the price information of the products.

The chemical batch plant operates under a finite timespan (H), from an initial time t_s to a final time t_f, and a finite optimal number of event points (E). There is set of unit operation times (T), totaling N_τ elements, comprised of a subset for stationary processes (τ_{Fix}) and a subset for dynamic processes (τ_{Dyn}).

It is desired to optimize an economic function (Z_{MIDO}) by finding an optimal scheduling plan (S_C), optimal control profiles (u) and unit operation times (τ_{Dyn}), which under a set of uncertain (stochastic) parameters (ψ_{Unc}), will hold dynamic feasibility of the flow-shop batch system. All these considerations result in the following MIDO problem:

$$\min_{u_j(t),\tau_{Dyn_j},s_{C_{e,j}}} Z_{MIDO}(x(t),u(t),\psi,t,s_C(e,\tau),c) \tag{1}$$

$$s.t.$$

$$f_{p,j}\big(x(t),\dot{x}(t),u(t),\psi,t,\tau,s_C(e,\tau)\big)=0, \quad \forall\, t,e\in E,p\in N_p,j\in N_E$$

$$h_{q,j}\big(x(t),\dot{x}(t),u(t),\psi,t,\tau,s_C(e,\tau)\big)\le 0, \quad \forall\, t,e\in E,q\in N_q,j\in N_E$$

$$k_{r,j}\big(x(t),\dot{x}(t),u(t),\psi,t,\tau,s_C(e,\tau)\big)=0, \quad \forall\, t,e\in E,r\in N_r,j\in N_E$$

$$u_{min}\le u_j(t)\le u_{max},\ \forall\, t,\ j\in N_{E_k},\ k\in N_{Pr}$$

$$\tau_{min}\le \tau_{Dyn_j}\le \tau_{max},\forall\, e,\ j\in N_{E_k},\ k\in N_{Pr}$$

$$x\in X\subseteq \mathbb{R}^{1\times N_x\times N_E},\ u\in U\subseteq \mathbb{R}^{1\times N_u\times N_E},\ c\in C\subseteq \mathbb{R}^{1\times N_C}$$

$$\psi_{Nom},\psi_{Unc}\in \Psi\subseteq \mathbb{R}^{1\times N_\psi},\ \tau_{Fix},\ \tau_{Dyn}\in T\subseteq \mathbb{R}^{1\times N_\tau}$$

$$s_{C_{e,j}}\in\{0,1\},\forall\, e\in E,\ j\in N_{E_k},\ k\in N_{Pr}$$

$$t\in[t_s,t_f],\ H=t_f-t_s$$

In problem (1), f_p usually represents the differential-algebraic equations (DAEs) that describe the model of a process p, $x(t)$ represents the states of the system, $u_j(t)$ represents the control variables required for unit j, $\tau_{Dyn,j}$ represents the unit operation time of unit j, $s_C(e,\tau)$ represents the set of integer and continuous decisions that specify the production schedule for the batch plant at event e. N_x, N_u & N_ψ, are the set of system states, the set of control variables and the set of system parameters, respectively.

Problem (1) can be casted as an infinite-dimensional stochastic MIDO problem, which is quite difficult to solve explicitly. Often, Problem (1) is reformulated as an MINLP by discretizing the differential equations. Due to the complex nature of such problems and the need of vast computational resources for their resolution, a decomposition method is proposed in this work. Thus, Problem (1) is reformulated as an scheduling problem, a dynamic optimization problem, Monte Carlo simulations and a dynamic unit time operation optimization problem. The resulting set of problems are solved iteratively using a back-off approach that was previously introduced by Koller and Ricardez-Sandoval (2017) and Valdez-Navarro and Ricardez-Sandoval (2019). The back-off approach introduces back-off terms that represent the variability of the system under the effect of random (stochastic) realizations in the uncertain parameters. The method makes use of the back-off terms to drive the system to a new feasible and attractive economic solution that can accommodate uncertainty. One limitation in previous back-off implementations is that unit operation times remained fixed during the calculations, which may lead to sub-optimal solutions since the back-off effect due to parameter uncertainty was not considered in allocation of the unit processing times.

3. METHODOLOGY

The key novelty of the present algorithm consists in the propagation of the variability observed in the controlled variables due to parametric uncertainty to the unit processing times, thus yielding scheduling and control decisions that will be less sensitive to stochastic parametric uncertainty. Hence, this approach will specify scheduling and control decisions, that combined with optimal unit operation times, results in dynamically feasible and economically attractive viable solutions (Z^*_{MIDO}). An illustration of the algorithm is shown in Figure 1. Each step of the algorithm is explained next.

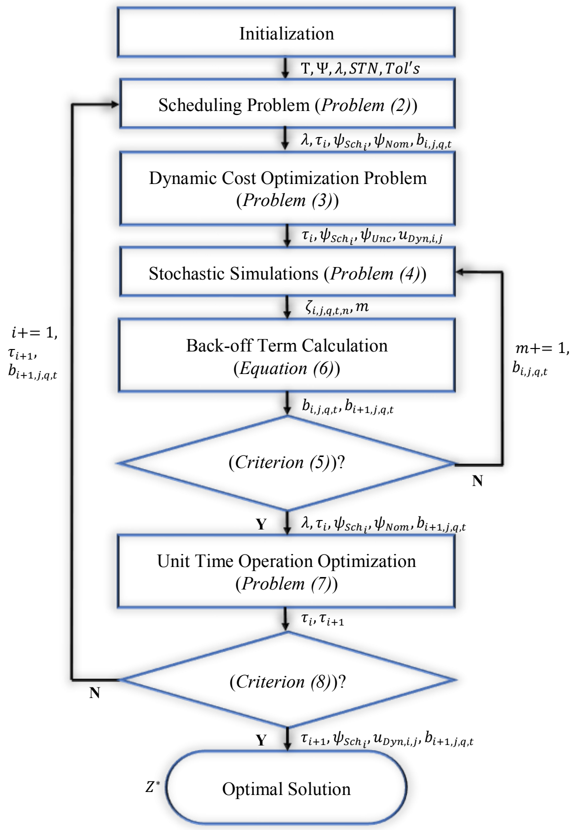

Figure 1. Proposed decomposition back-off algorithm.

3.1 Initialization

The sets T and Ψ must be initialized; also, initial values are needed for the specification of the State-Task Network (STN) for the scheduling problem (i.e. E, H, ρ_0, P, C_0). Moreover, it is necessary to define the probabilistic distribution function (PDF) and their corresponding parameters (η) that will describe each parameter conforming ψ_{Unc} (i.e. for an element w: $\psi_{Unc_w}=PDF_w(\eta_w)$. These data can be obtained from process heuristics or from historical data. Tolerance criteria (Tol_{SS} & Tol_{BO}) are also required for initialization. The iteration index for the algorithm is also set, i.e. $i = 0$.

3.2 Scheduling Problem

A continuous-time formulation and a State-Task Network (STN) are used in this work for the reformulation of the scheduling problem shown in Problem (1). A continuous-time formulation allows for a variable partition of time and the allocation of processes of varying time lengths while, in general, lowering computational costs compared to a uniform discrete-time approach (Floudas and Lin, 2004). STN representations are preferred because of their ability to describe multiproduct-multipurpose chemical batch chemical plants and their lack of ambiguity (Floudas and Lin, 2004). The continuous-time scheduling formulation is represented by the following MILP problem:

$$\max_{W_{i,k,e}, Y_{i,j,e}} Z_{Sch}\left(c_{i,k,j}, p_s, \rho_{i,k,s}^{in}, \rho_{i,k,s}^{out}, d_{i,s,e}, E_i, H\right) \quad (2)$$

$$s.t.$$

$$\sum_{k \in N_{Pr_j}} W_{i,k,e} \leq Y_{i,j,e}, \forall j \in N_E, e \in E \quad (2a)$$

$$W_{i,k,e} B_{Min_{k,j}} \leq B_{i,k,j,e} \leq W_{i,k,e} B_{Max_{k,j}} \quad (2b)$$
$$\forall k \in N_{Pr}, j \in N_{E_k}, e \in E$$

$$ST_{i,s,e} = ST_{i,s,e-1} - d_{i,s,e} \quad (2c)$$
$$+ \sum_{k \in N_{Pr_s}} \rho_{i,k,s}^{Out} \sum_{j \in N_{E_k}} B_{i,k,j,e-1}$$
$$- \sum_{k \in N_{Pr_s}} \rho_{i,k,s}^{In} \sum_{j \in N_{E_k}} B_{i,k,j,e},$$
$$\forall s \in S, e \in E$$

$$ST_{i,s,e} \leq O_s, \forall s \in S, e \in E \quad (2d)$$

$$Q_{i,j,e} = Q_{i,j,e-1} + \sum_{k \in N_{Pr_j}} B_{i,k,j,e} \quad (2e)$$
$$- \sum_{k \in N_{Pr_j}} \sum_{s \in S_k^{out}} \rho_{i,k,s}^{out} B_{i,k,j,e-1},$$
$$Q_{i,j,e_f} = 0, \forall j \in N_E, e \in E$$

$$\sum_{e \in E} d_{i,s,e} \geq r_s \quad \forall s \in S \quad (2f)$$

$$T_{i,k,j,e}^F = T_{i,k,j,e}^S + \tau_{i,k} W_{i,k,e}, \forall k \in N_{Pr_j}, j \in N_E, \quad (2g)$$
$$e \in E$$

$$T_{i,k,j,e}^F \geq T_{i,k,j,e}^S, \forall k \in N_{Pr_j}, j \in N_E, e \in E \quad (2h)$$

$$T_{i,k,j,e+1}^S \geq T_{i,k,j,e}^F, \forall k \in N_{Pr_j}, j \in N_E, e \in E \quad (2i)$$

$$T_{i,k,j,e+1}^F \geq T_{i,k,j,e}^F, \forall k \in N_{Pr_j}, j \in N_E, e \in E \quad (2j)$$

$$T_{i,k,j,e+1}^S \geq T_{i,k,j,e}^S, \forall k \in N_{Pr_j}, j \in N_E, e \in E \quad (2k)$$

$$T_{i,k,j,e}^F \leq H, \forall k \in N_{Pr_j}, j \in N_E, e \in E \quad (2l)$$

$$T_{i,k,j,e}^S \leq H, \forall k \in N_{Pr_j}, j \in N_E, e \in E \quad (2m)$$

$$T_{i,k,j,e_f}^F = H, \forall k \in N_{Pr_j}, j \in N_E, e \in E \quad (2n)$$

$$T_{i,k,j,e+1}^S \geq T_{i,l,j,e}^F - H(1 - W_{i,l,e}) \quad (2o)$$
$$\forall j \in N_E, k \in N_{Pr_j}, l \in N_{Pr_j}, k \neq l, e \in E, e \neq e_f$$

$$where$$
$$c_{i,k,j} \in C_i, \forall k \in N_{Pr_j}, j \in N_E$$
$$p_s \in P, r_s \in R, \forall s \in S$$
$$\rho_{i,k,s} \in \rho_i, \forall k \in N_{Pr}, s \in S$$

In Problem (2) the objective is to maximize the profit from producing a variety of products by implementing their recipes. Note that other objective functions can be implemented. $c_{i,k,j}$ represents the cost of task k in unit j at the i^{th} iteration, P_s is the sale price of state s, E is the number of event points. Eq. (2a) represents the allocation constraints where $W_{i,k,e}$ is set to zero unless task k at event e is taking place in unit j at the i^{th} iteration, also, this constraint depends on the value of $Y_{i,j,e}$, which represents the assignment of unit j at event e at the i^{th} iteration (with a value of 1). Eq. (2b) represents the capacity constraint, where $B_{i,k,j,e}$ is the material holdup of unit j while processing task k at event e.. Eq. (2c) represents the state material balances. $ST_{i,s,e}$ is the total quantity of state s at event e whereas $\rho_{i,k,s}^{In}$ and $\rho_{i,k,s}^{Out}$ represent the proportion of state s that is consumed or produced by task k, respectively. Eq. (2d) ensures that the quantity produced by each state is not greater than its capacity O_s. Eq. (2e) is the material balance inside each unit j with the condition that at the end of the last event e_f, must be equal to zero as all units must be emptied (no remaining material inside the processing units is allowed). Eq. (2f) represents the market demand constraints, where r_s is the total demand of state s and $d_{i,s,e}$ is the demand satisfied of such state at event e. Eq. (2g) to Eq. (2n) are time logic constraints, i.e. they represent the time at which a task k starts to take place at unit j and in which event e takes place; they also enforce that no unit can be operated beyond the time horizon H. Eq. (2o) ensures the consecutiveness in the occurrence of two tasks sharing the same unit. Note that in problem (2), the parameters in the sets C_i and ρ_i change at each iteration i in accordance with the information gathered from the previous iteration(s).

3.3 Dynamic Cost Optimization Problem

The set of scheduling decisions β_{Sch_i} ($W_{i,k,e}$ and $Y_{i,j,e}$) can be obtained from the solution of Problem (2) ($Z_{Sch_i}^*$). This represents the key inputs required for the formulation of a dynamic cost optimization problem. In particular, the nonlinear dynamic optimization Problem (3) aims to find the control actions $u_{i,j,t}$ for each unit j at time t in the i^{th} iteration that maximize the profit and is subjected to the scheduling decisions β_{Sch_i} found from Problem (2), i.e.

$$\max_{u_{i,j,t}} Z_{Dyn}(x(t), \dot{x}(t), u(t), \Psi, t, \tau_i, C_i) \quad (3)$$

$$s.t.$$

$$f_{p,j}\left(x(t), \dot{x}(t), u(t), \beta_{Sch_i}, \psi_{Nom}, t, \tau_{i,}\right) = 0, \quad (3a)$$
$$\forall t, p \in N_p, j \in N_E$$

$$h_{q,j}\left(x(t), \dot{x}(t), u(t), \beta_{Sch_i}, \psi_{Nom}, t, \tau_i\right) \quad (3b)$$
$$\pm \lambda b_{i-1,j,q,t} \leq 0, \forall t, q \in N_q, j \in N_E$$

$$where$$
$$\psi_{Nom} \in \Psi, \tau_i \in T$$

In Problem (3), the back-off terms $b_{i,j,q,t}$ represent the deviation of system from the nominal point under realizations in uncertain model parameters at the inequality constraint q of unit j at time t at the i^{th} iteration. More details about the back-off terms is provided in subsection 3.5. Consideration of the back-off terms in Eq. (3b) forces the system to find control decisions that will account for this back-off while ensuring dynamic feasibility. Note that back-off terms at the initial iteration ($i = 0$) have a value equal to zero. As shown in Eq. (3b), the back-off terms are preceded by a multiplier-factor λ, which can be thought as the level confidence given to each of the back-off terms. Note that Valdez-Navarro and Ricardez-Sandoval (2019) studied in a previous work the effects of choosing the value of the λ multiplier.

3.4 Stochastic Simulations

Let $Z^*_{Dym_i}$ be the solution obtained from Problem (3) and $u_{Dyn_{i,j}}$ the corresponding optimal control profiles obtained under the effect of back-off terms identified from the previous iteration. Hence, such control actions are not guaranteed to remain feasible under uncertainty.

In this step, the resilience of $u_{Dyn_{i,j}}$ to drive the system to feasible solutions is evaluated under a set of n stochastic realizations in the uncertain parameters ($\psi_{Unc_{i,n}}$), i.e. the value of ψ_{Unc} changes at each realization n. The realization in ψ_{Unc} are taken from their corresponding probability function (PDF) for each uncertain parameter and specified in the initialization step. This step is needed to generate statistical data that will allow for the recalculation of back-off terms at the current iteration. The problem under consideration is as follows:

$$\max \zeta_{i,j,q,t,n} = h_{q,j,n}\left(x(t), \dot{x}(t), u_{Dyn_i}, \psi_{Unc_{i,n}}, t, \tau_{i,}\right) \tag{4}$$

$$s.t.$$

$$f_{p,j,n}\left(x(t), \dot{x}(t), u_{Dyn_i}, \psi_{Unc_{i,n}}, t, \tau_{i,}\right) = 0, \quad \forall\, t, p \in N_p, j \in N_E \tag{4a}$$

$$where$$

$$\psi_{Unc_{i,n}} \in \Psi, \mathrm{\tau_i} \in \mathrm{T}$$

The considerations required for Problem (4) are as follows: i) only the mechanistic models ($f_{p,j,n}$) are enforced; ii) control variables ($u_{Dyn_{i,j}}$) remain fixated; iii) only the feasibility of the system is assessed under different realizations in the uncertain parameters; iv) each uncertain parameter in $\psi_{Unc_{i,n}}$ is described by a PDF, thus, the values used while solving Problem (4) are selected from Monte Carlo (MC) sampling techniques. Problem (4) is solved N_{MC} times, which is the total of stochastic realizations considered. N_{MC} is unknown a priori as problem (4) has to be solved in batches of n realizations of $\psi_{Unc_{i,n}}$ until a user-defined criterion is met.

Criterion (5) quantifies the deviations in the back-off term between the m^{th} and $m-1^{th}$ data populations. Note that each population m is composed of $n*m$ realizations in the uncertain parameters. This criterion makes this step repeat until the errors between the back-off terms in the actual data set (i.e. population m) and the previous data collected (i.e. population $m-1$) is below a user defined tolerance. Note that population m includes the information of previous populations and that N_{MC} is equal to the number of data points in the last m^{th} population. Also, note that Criterion (5) can only be enforced when $m \geq 2$ and that such criterion must be satisfied by all q constraints. The specific procedure to estimate the back-off terms shown in Criterion (5) is presented in subsection 3.5.

$$\left|1 - b_{i,j,q,t,m-1}/b_{i,j,q,t,m}\right| \leq Tol_{SS} \quad \forall\, \mathrm{t}, \mathrm{j} \in N_E, \mathrm{q} \in N_q \tag{5}$$

3.5 Back-Off Term Calculation

A back-off term ($b_{i,j,q,t}$) is the representation of the deviation in the q^{th} constraint function ($\zeta_{i,j,q,t,n}$) at a time t for a unit j at the i^{th} iteration for each stochastic simulation n in the uncertain parameters. The introduction of $b_{i,j,q,t}$ into constraints h_q is to search for a solution capable of accommodating uncertainty, backed off from the optimal solution at nominal model parameters (Koller et al., 2018). Note that there is back-off term for each inequality q at each time point t, i.e.

$$b_{i+1,j,q,t} = \sqrt{\frac{1}{N_{MC}} \sum_{n=1}^{N_{MC}} \left[\zeta_{i,j,q,t,n} - \frac{1}{N_{MC}} \sum_{n=1}^{N_{MC}} \zeta_{i,j,q,t,n}\right]^2} \quad \forall\, \mathrm{j} \in \mathrm{N}_{\mathrm{E}_{i,q}}, \ \mathrm{q} \in N_{q_i}, \ t \in [0,1] \tag{6}$$

Eq (6) represents the calculation of the normal standard deviation for discrete random variables, which is used for the calculation of the back-off terms in this work. Eq (6) may vary correspondingly to the statistical distribution of $\zeta_{i,j,q,t,n}$. Note that it is Eq. (6) that is used to calculate the back-off terms at each m population in the procedure described in subsection 3.4. Also, note that the iteration index i has been updated in Eq. (6) to indicate that these back-off terms have been updated and may be used in subsequent calculations. In this work, it is assumed that the data used for the back-off terms calculation, $\zeta_{i,j,q,t,n}$, follows a statistical distribution that can be approximated to a normal distribution.

3.6 Unit Operation Times Optimization Problem

Since the back-off terms represent the degree of variability that the constraints need to accommodate using an optimal control profile, in this step, such variability is used to determine the optimal operation times for each unit j. Problem (7) is set to determine the minimum time required for each unit to achieve their corresponding production goals under parameter uncertainty, which is expressed through the back-off terms.

$$\min_{\tau_{Dyn_{i+1,j}}} Z_{UOT}(x(t), \dot{x}(t), u(t), \Psi, t, \tau_{i+1}, C_i) \tag{7}$$

$$s.t.$$

$$f_p\left(x(t), \dot{x}(t), u(t), \beta_{Sch_i}, \psi_{Nom}, t, \tau_{Dyn_{i+1,j}}\right) = 0, \quad \forall\, t, p \in N_{p_i} \tag{7a}$$

$$h_q\left(x(t), \dot{x}(t), u(t), \beta_{Sch_i}, \psi_{Nom}, t, \tau_{Dyn_{i+1,j}}\right) \pm \lambda b_{i+1,j,q,t} \leq 0, \forall\, t, \ j \in N_{E_i}, \ q \in N_{q_i} \tag{7b}$$

$$\tau_{Min_j} \leq \tau_{Dyn_{i+1,j}} \leq \tau_{Max_j}, \ \tau_{Dyn_{i+1,j}} \in \tau_{i+1}, \quad \forall\, j \in N_{E_i}$$

$$where$$

$$\psi_{Nom} \in \Psi, \tau_{i+1} \in \mathrm{T}$$

Let $Z^*_{UOT_i}$ be the solution for problem (7), then $\tau_{i+1} = \left\{\tau_{Dyn_{i+1}}, \tau_{Nom}\right\}$ is the set of all the unit operation times ($\tau_{i+1} \in Z^*_{UOT_i}$) under model parameter uncertainty. Once the optimization of the unit operation time has been performed, the variation between the back of terms used in the i^{th} iteration ($b_{i,j,q,t}$), and those calculated in the current iteration ($b_{i+1,j,q,t}$) is set as the criterion that will terminate the algorithm if such deviation is lesser than a user-defined tolerance (Tol_{BO});

otherwise, the algorithm proceeds with the next iteration, as shown in Figure 1. This criterion is defined as follows:

$$\left|1 - b_{i-1,j,q,t}/b_{i,j,q,t}\right| \leq Tol_{BO}, \quad \forall\, t, j \in N_E, q \in N_q \tag{8}$$

If Criterion (8) is met, a solution Z^* that is composed by the control decisions u_{Dyn}, unit operation times τ_{Dyn} and process scheduling decisions β_{Sch}, that accommodates the variability in the uncertain model parameters (ψ_{Unc}), has been found.

4. CASE STUDY

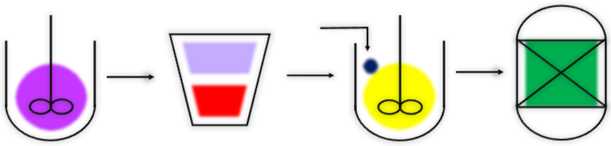

Figure 2. Case Study Process Scheme.

A modified version of the chemical batch plant presented by Chu and You (2013) has been used to test the performance of the proposed back-off algorithm. As shown in Figure 2, the chemical batch plant consists of 4 batch processes: a set of chemical reactions I (RI), a filtration process (FI), a set of chemical reactions II (RII) and a separation process (SI), i.e. $N_{Pr} = \{RI, RII, FI, SI\}$. The time horizon ($H$) of operation for this plant has been set to 13 h. To simplify the analysis, one unit for each process has been considered, though multiple units for each process could be considered. The general process consists on substance A being transformed into product B in process RI, while the temperature of the reactor is controlled. Then, the mixture containing substance B is purified in process FI. Substance B is then stored in the reactor where process RII and D is fed in a controlled fashion to obtain product E. In SI, the mix containing species B and E (desired product) is separated from the mix of D and F. Process FI and SI are stationary and assumed to achieve perfect separation whereas RI and RII are time dependent processes; thus, their corresponding unit operation times (τ_{Dyn}^{RI} & τ_{Dyn}^{RII}) will be obtained from optimization. The following set of equations describe the dynamic process RI:

$$A \overset{r_1}{\rightarrow} B \overset{r_2}{\rightarrow} C \tag{9}$$
$$\frac{dC_A}{dt} = -r_1, \frac{dC_B}{dt} = r_1 - r_2$$
$$\frac{dT_R}{dt} = -\frac{\Delta H_1 r_1 + \Delta H_2 r_2}{\rho_R c_R} + \frac{UA_j(T_J - T_R)}{V_R \rho_R c_R}$$
$$\frac{dT_J}{dt} = \frac{F_{Hot}(T_{Hot} - T_J)}{V_J} + \frac{F_{Cold}(T_{Cold} - T_J)}{V_J} + \frac{UA_j(T_R - T_J)}{V_R \rho_R c_R}$$
$$r_1 = k_1 e^{-E_1/T_R} C_A, r_2 = k_2 e^{-E_2/T_R} C_B$$
$$C_A(0) = C_{A_0}, C_B(0) = C_{B_0},$$
$$T_R(0) = T_{R_0}, T_J(0) = T_{J_0}$$
$$C_B(t_f) \geq C_{B_{Fix}}, T_R(t_f) \leq T_{R_{Fix}}$$
$$u(t) = [F_{Hot} \;\; F_{Cold}]$$

Similarly, for process RII:

$$B + D \overset{r_3}{\rightarrow} E, 2D \overset{r_4}{\rightarrow} F \tag{10}$$
$$\frac{dV_R}{dt} = F_{Feed}$$
$$\frac{dC_B}{dt} = -r_3 - \frac{F_{Feed}}{V_R} C_B$$
$$\frac{dC_D}{dt} = -r_3 - 2r_4 + \frac{F_{Feed}}{V_R}(C_{D_{Feed}} - C_D)$$
$$\frac{dC_E}{dt} = r_3 - \frac{F_{Feed}}{V_R} C_E$$
$$\frac{dC_F}{dt} = r_3 - \frac{F_{Feed}}{V_R} C_F$$
$$r_3 = k_3 C_B C_D, r_4 = k_4 C_D^2$$
$$V_R(0) = V_{R_0}, C_A(0) = C_{A_0},$$
$$C_B(0) = C_{B_{RI}}, C_C(0) = C_{C_0},$$
$$V_R(t_f) C_E(t_f) \geq V_{Fix} C_{E_{Fix}}, V_R(t_f) \leq V_{R_{Fix}}$$
$$V_R(t_f) C_F(t_f) \leq V_{Fix} C_{F_{Fix}}$$
$$u(t) = [F_{Feed}]$$

Table 1 list key parameters and variables used for this case study; the rest of the parameters can be found in Chu and You (2013). This work assumes that k_{AB} and k_{BC} follow a normal distribution with expected value as shown in Table 1 and with a standard deviation equivalent to 5% of their expected values.

Table 1. Process Parameters and Variables.

Variable Name	Value	Description
$E_{A\rightarrow B}$ $[K]$	4500	Activation Energy
$E_{B\rightarrow C}$ $[K]$	8250	Activation Energy
$p_{F_{Cool}}$ $[m.u/m^3]$	0.5	Aux. Serv. Price
$p_{F_{Hot}}$ $[m.u/m^3]$	0.5	Aux. Serv. Price
$p_{F_{Feed}}[m.u./kmol]$	50	Raw Feed Price
$p_A[m.u./kmol]$	100	Raw Material Price
$p_{Waste}[m.u./kmol]$	1000	Waste Cost
$p_{Pure}[m.u./kmol]$	10000	Product Price
$p_{Impure}[m.u./kmol]$	1000	Sub-product Cost
$C_{D_{Feed}}$ $[kmol/m^3]$	10	Feed Concentration
$C_{F_{Fix}}$ $[kmol/m^3]$	0.15	Final Concentration
k_{AB} $[h^{-1}]$	1E7	Kinetic Velocity
k_{BC} $[h^{-1}]$	1E10	Kinetic Velocity
λ	2	Confidence

The profit function for problem (3), i.e. the dynamic optimization problem, is as follows: $Z_{Dyn} = \sum_k^{N_{Pr}} \sum_j^{N_{Ek}} c_{k,j}$. This function involves the cost of auxiliary services for RI ($-c_{RI} = p_{F_{Hot}} \int_0^{\tau_{Dyn}^{RI}} F_{Hot}(t)dt + p_{F_{Cool}} \int_0^{\tau_{Dyn}^{RI}} F_{Cool}(t)dt$), the cost for raw species A at the beginning of process RI ($-c_{A_{RI}} = p_A C_A(t)|_{t=0}$), the cost for the waste generated in FI ($-c_{FI} = p_{Waste}(C_A(t) + C_C(t))|_{t=\tau_{Dyn}^{RI}}$), the cost for species D fed into process RII ($-c_{RII} = p_{F_{Feed}} V_R(t) C_F(t)|_{t=\tau_{Dyn}^{RII}}$), the revenues for the mixture of D and F ($c_{SI_1} = p_{Pure}(C_D(t) + C_F(t))|_{t=\tau_{Dyn}^{RII}}$), and the cost for the mixture of B and E in process SI ($-s_{SI_2} = p_{Impure}(C_B(t) + C_E(t))|_{t=\tau_{Dyn}^{RII}}$). The profit function used in the scheduling problem (2) ($Z_{Sch} = c_{ST} + c_{Op}$) involves the costs associated with the operation ($c_{k,j}$) of unit j to realize task k at event e ($c_{Op} = -\sum_e^E \sum_k^{N_{Pr}} \sum_j^{N_{Ek}} W_{k,e} \tau_j c_{k,j}$) and the cost/revenue of the material generated/consumed ($c_{ST} = \sum_e^E \sum_s^S d_{s,e} c_s$, where $c_s < 0$ for costs and $c_s > 0$ for revenues). Additional details can be found in Chu and You (2013).

5. RESULTS

The case study was implemented using Pyomo optimization suite within Python 3.7. The Interior Point algorithm IPOPT™ was used to solve Problems (3), (4) and (7). CPLEX was used to solve Problem (2). The model was solved in a PC with an Intel® Core™ i7-8700 CPU @ 3.2 GHz and 16 GB of RAM. For comparison purposes, the present case study was solved using the algorithm presented in this work and that proposed by Valdez-Navarro and Ricardez-Sandoval (2019) where unit operations times remain fixed during the calculations.

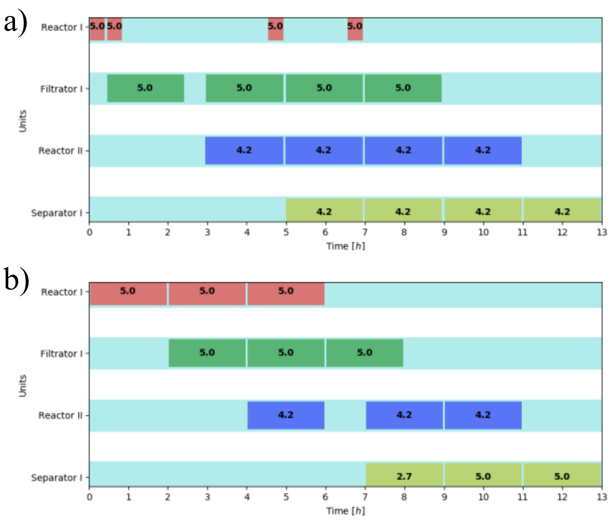

Figure 3. Scheduling Plan: *a*) Proposed algorithm, *b*) Valdez-Navarro's algorithm.

As shown in Figure 3, the proposed algorithm can accommodate another batch sequence by finding new unit operations times that increase plant production (material processing batch size is shown inside each unit assignment in the figure). While all the unit operation times were set to 2h for Valdez-Navarro's algorithm (Fig. 3b), it can be observed that the values τ_{Dyn}^{RI} and τ_{Dyn}^{RII} for the present approach are 0.436h and 2.017h, respectively (Fig. 3a). The operation regimes found by the present algorithm are more economically expensive, as more control actions are required to maintain the dynamic feasibility (the control profiles are not shown for brevity). Nevertheless, there is an increase in production for the case in Fig. 3a) which increases the profits by a 42% (90,386 m.u. for the proposed algorithm compared to 63,369 m.u. obtained from Valdez-Navarro's algorithm). Regarding CPU times, each iteration of the present algorithm requires on average 8 h, with 3 iterations required to solve the present case study. On the other hand, 2 iterations and 4 h per iteration were required by Valdez-Navarro's algorithm. Note that the selection of the tolerance parameters (Tol_{SS} & Tol_{BO}) is problem-specific and will impact the algorithm's computational costs. In this work, both Tol_{SS} & Tol_{BO} were set to 0.0025, which were adequate as they returned acceptable results in reasonable CPU times.

6. CONCLUSION

A new back-off algorithm for the integration of scheduling and control of multi-unit, multi-product chemical batch plants under stochastic uncertainty was presented. The key idea is to introduce a formulation that searches for the optimal unit processing times using back-off terms, which reflect process variability under uncertainty. The results show that the present algorithm can improve profits by choosing optimal unit operation times. Future work will explore the implementation of the present algorithm for the simultaneous scheduling, design and control of batch systems under uncertainty. Also, an approach that simultaneously computes unit operation times and optimal control profiles will be explored.

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