Dynamic Optimization in the Batch Chemical Industry

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Abstract

Dynamic optimization of batch processes has attracted more attention in recent years since, in the face of growing competition, it is a natural choice for reducing production costs, improving product quality, and meeting safety requirements and environmental regulations. Since the models currently available in industry are poor and carry a large amount of uncertainty, standard model-based optimization techniques are by and large ineffective, and optimization methods need to rely more on measurements.

In this paper, various measurement-based optimization strategies reported in the literature are classified. A new framework is also presented, where important characteristics of the optimal solution that are invariant under uncertainty are identified and serve as references to a feedback control scheme. Thus, optimality is achieved by tracking with no numerical optimization required on-line. When only batch-end measurements are available, the proposed method leads naturally to an efficient batch-to-batch optimization scheme. The approach is illustrated via simulation of a semi-batch reactor in the presence of uncertainty.

Keywords

Dynamic optimization, Optimal control, Batch chemical industry, On-line optimization, Batch-to-batch optimization, Run-to-run optimization.

Introduction

Batch and semi-batch processes are of considerable importance in the chemical industry. A wide variety of specialty chemicals, pharmaceutical products, and certain types of polymers are manufactured in batch operations. Batch processes are typically used when the production volumes are low, when isolation is required for reasons of sterility or safety, and when frequent changeovers are necessary. With the recent trend in building small flexible plants that are close to the markets of consumption, there has been a renewed interest in batch processing (Macchietto, 1998).

From a process systems point of view, the key feature that differentiates continuous processes from batch and semi-batch processes is that the former have a steady state, whereas the latter are inherently time-varying in nature (Bonvin, 1998). This paper considers batch and semi-batch processes in the same manner and, thus herein, the term 'batch processes' includes semi-batch processes as well.

The operation of batch processes typically involves following recipes that have been developed in the laboratory. However, owing to differences in both equipment and scale, industrial production almost invariably necessitates modifications of these recipes in order to ensure productivity, safety, quality, and satisfaction of operational constraints (Wiederkehr, 1988). The 'educated trials' method that is often used for recipe adjustment is based on heuristics and results in conservative profiles. Conservatism is necessary here to guarantee feasibility despite process disturbances.

To shorten the time to market (by bypassing an elaborate scale-up process) and to reduce operational costs (by reducing the conservatism), an optimization approach is called for, especially one that can handle uncertainty explicitly. Operational decisions such as temperature or feed rate profiles are then determined from an optimization problem, where the objective is of economic nature and the various technical and operational constraints are considered explicitly. Furthermore, due to the repetitive nature of batch processes, these problems can also be addressed on a batch-to-batch basis.

The objectives of this paper are threefold: i) address the industrial practice prevailing in the batch specialty chemical industry and discuss the resulting optimization challenges, ii) review the dynamic optimization strategies available for batch processes, with an emphasis on measurement-based techniques, and iii) present a novel scheme that uses the available process measurements directly (i.e., without the often difficult step of model refinement) towards the goal of optimization. Accordingly, the paper has three major parts:

- *Industrial perspectives in batch processing:* The major operational challenges aim at speeding up process/product development, increasing the productivity, and satisfying safety and product quality requirements (Allgor et al., 1996). These tasks need to be performed in an environment characterized by a considerable amount of uncertainty and the presence of numerous operational and safety-related constraints. The measurements available could be used to help meet these challenges.
- *Optimization strategies for batch processes:* These are reviewed and classified according to: i) whether uncertainty is considered explicitly, ii) whether measurements are used, iii) whether a model is used to guide the optimization. The type of measurements used for optimization (on-line, off-line) adds another dimension to the classification.
- *Invariant-based optimization scheme:* New insights into the optimal solution for a class of batch processes have led to an alternative way of dealing with uncertainty. It involves: i) the off-line characterization of the optimal solution using a simplified model, ii) the selection of signals that are invariants to uncertainty, and iii) a model-free implementation by tracking these invariants using a limited number of measurements. This results in a model-free though measurement-based implementation that is quite robust towards uncertainty. An interesting feature of this framework is that it permits naturally to combine off-line data from previous batches with on-line data from the current batch.

The paper is organized as follows. The industrial perspectives in batch processing are presented first. The next section briefly reviews the optimization strategies available for batch processes and proposes a classification of the methods. The invariant-based optimization framework is then developed and an example is provided to illustrate the theoretical developments. Conclusions are drawn in the final section.

Industrial Perspectives in Batch Processing

It is difficult to address in generic terms the perspectives prevailing in the batch chemical industry since the processing environments and constraints differ considerably over the various activities (specialty chemicals, pharmaceuticals, agro and bio products, etc.). Thus, the situation specific to the production of intermediates in the specialty chemical industry will be emphasized in this section. The customer – typically an end-product manufacturer – often generates competition between several suppliers for the production of a certain product. The suppliers need to investigate the synthesis route and design an appropriate production process. The competition forces the suppliers to come up, under considerable time pressure, with an attractive offer (price/kg) if they want to obtain the major share of the deal.

Batch processes are usually carried out using relatively standardized pieces of equipment whose operating conditions can be adjusted to accommodate a variety of products. The working environment that will be considered is that of multi-product plants. In a multi-product plant, a number of products are manufactured over a period of time, but at any given time, only one product is in the process. The sequence of tasks to be carried out on each piece of equipment such as heating, cooling, reaction, distillation, crystallization, drying, etc. is pre-defined, and the equipment item in which each task is performed is also specified (Mauderli and Rippin, 1979).

Operational Objectives

The fundamental objective is of economic nature. The investment (in time, personnel, capital, etc.,) should pay off, as the invested capital has to compare favorably with other possible investments. This fundamental objective can in turn be expressed in terms of technical objectives and constraints, which are presented next.

- *Productivity:* This is the key word nowadays. However, high productivity requires stable production so as to reduce the amount of corrective manual operations that are costly in terms of production time and personnel. Reducing the time necessary for a given production is particularly interesting when the number of batches per shift can be increased. In multi-product plants, however, equipment constraints (bottlenecks) and logistic issues often limit productivity.
- *Product quality:* Quality is often impaired by the appearance of small amounts of undesired by-products. The presence of impurities (also due to recycled solvents) is very critical since it can turn an acceptable product into waste. Removing impurities is often not possible or can significantly reduce throughput. Also, from an operational, logistic and regulation point of view, it is often not possible to use blending operations in order to achieve the desired average quality.
  Reproducibility of final product composition despite disturbances and batch-to-batch variations is important when the process has to work closely to some quality limit (for example, when the quality limits are tight). Improving the selectivity of an already efficient process is often not seen as a critical factor. However, when the separation of an undesirable by-product is difficult, the selectivity objective may be quite important.
- *Safety aspects:* The safety aspects (runaway, contamination, etc.) are of course very important. Safety requirements can lead to highly conservative operation. Here, the real obstacle is the lack of on-line information. If information about the state of the process were available, the process engineer would know how to guarantee safety or react in the case of a latent problem. Thus, the difficulty results from a measurement limitation and not from a lack of operational knowledge.
- *Time-to-market:* The economic performance is strongly tied to the speed at which a new product/process can be developed. The product lifetime of specialty chemicals is typically shorter than for bulk chemicals. Since the production in campaigns reduces the time to learn, it is necessary to learn quickly and improve the productivity right away. After a couple of years, a profitable new product may become a commodity (of much lesser value), for which the development of a second-generation process is often considered.
  Nowadays, there is a trend in the specialty chemical industry to skip pilot plant investigations unless the process is difficult to scale up. The situation is somewhat different in pharmaceuticals production, where pilot plant investigations are systematically used since they also serve to produce the small 'first amounts' needed.

Industrial Practice

Though the problem of meeting the aforementioned objectives could be solved effectively as an optimization problem, there have been only a few attempts in industry to optimize operations through mathematical modeling and optimization techniques. The recipes are developed in the laboratory in such a way that they can be implemented safely in production. The operators then use heuristics gained from experience to adjust the process periodically (whenever this is allowed), which leads to slight improvements from batch to batch (Verwater-Lukszo, 1998). The stumbling blocks for the use of mathematical modeling and optimization techniques in industrial practice have been partly organizational and partly technical.

Organizational issues. At the organizational level, the issues are as follows:

- *Registration:* Producers of active compounds in the food and pharmaceuticals areas have to pass through the process of registration with the Food and Drug Administration. Since this is a costly and time-consuming task, it is performed simultaneously with R&D for a new production process. Thus, the main operational parameters are fixed within specified limits at an early stage of the development. Since the specifications provided by the international standards of operation (GMP) are quite tight, there is very little room for maneuver left. It is important to stress that the registration is tied to both product *and* process.
- *Multi-step process:* In the R&D phase of a large multi-step process, different teams work on different processing steps. Often, each team tries to optimize its process subpart, thereby introducing a certain level of conservatism to account for uncertainty. Consequently, the resulting process is the sum of conservatively designed subparts, which often does not correspond to the optimum of the global process!

- *Role of control and mathematical optimization:* In many projects, control is still considered to be a standard task that has to be performed during the detailed engineering phase and not as a part of the design phase of the process. It is like 'painting' a controller or an optimizer once the process has been built. At this late stage, there is so much conservatism and robustness in the system that it does not require a sophisticated control strategy. However, the performance may still be far from being optimal.

All these organizational problems can be resolved by resorting to 'global thinking'. It has become a challenge for both project leaders and plant managers to make chemists and engineers think and act in a global way. It is done through fostering interdisciplinary teamwork and simultaneous rather than sequential work for process research, development and production (R&D&P). The objective is a globally optimal process and not simply the juxtaposition of robust process subparts. Team work amounts to having R&D&P solutions worked out simultaneously by interdisciplinary teams consisting of a project leader, chemists, process engineers, production personnel and specialists for analytics, simulation, statistics, etc.

Technical issues. The main technical issues relate to modeling and measurements, the presence of both uncertainty and constraints, and the proper use of the available degrees of freedom for process improvement. These are addressed next.

- *Modeling:* In the specialty chemical industry, molecules are typically more complex than in the commodity industry, which often results in complex reaction pathways. Thus, it is illusory to expect constructing detailed kinetic models. The development of such models may exceed one man-year, which is incompatible with the objectives of batch processing. So, what is often sought in batch processing, is simply the ability to predict the batch outcome from knowledge of its initial phase.

  Modern software tools such as Aspen Plus, PRO/II, or gPROMs have found wide application to model continuous chemical processes (Marquardt, 1996; Pantelides and Britt, 1994). The situation is somewhat different in batch specialty chemistry. Though batch-specific packages such as Batch Plus, BATCH-FRAC, CHEMCAD, BatchCAD, or BaSYS are available, they are not generally applicable. Especially the two important unit operations, reaction and crystallization, represent a considerable challenge to model at the industrial level.

  For batch processes, modeling is often done empirically using input/output static models on the basis of statistical experimental designs. These include operational variables specified at the beginning of the batch and quality variables measured at the end of the batch. Time-dependent variables are not considered beyond visual comparison of measured profiles. Sometimes the model is a set of simple linguistic rules based on experience, e.g. when 'low' then 'bad'. Occasionally, the model consists of a simple energy balance, or the main dynamics are expressed via a few ordinary differential equations. The modeling objective is not accuracy but rather the ability to semi-quantitatively describe the major tradeoffs present in the process such as the common one between quality and productivity in many transformation and separation processes. For example, an increase in reflux ratio improves distillate purity but reduces distillate flow rate; or a temperature increase can improve the yield at the expense of selectivity in a chemical reaction system.

- *Measurements:* Quality measurements are typically available at the end of the batch *via*, for example, off-line chromatographic methods (GC, HPLC, DC, IC). In addition, physical measurements such as temperature, flow, pressure, or pH may be available on-line during the course of the batch. However, they are rather unspecific with respect to the key variables (concentrations) of the chemical process. Other on-line measurements such as conductivity, viscosity, refractive index, torque, spectroscopy, and calorimetry are readily available in the laboratory, but rarely in production. Pseudo on-line GC and HPLC are less effective in batch processing than with continuous processes due to relatively longer measurement delays.

  On-line spectroscopy (FTIR, NIR, Raman) has opened up new possibilities for monitoring chemical processes (McLennan and Kowalski, 1995; Nichols, 1988). These techniques rely on multivariate calibration for accurate results, i.e., the spectral measurements need to be calibrated with respect to known samples containing all the absorbing species. Though on-line spectroscopy is getting more common in the laboratory, the transfer of many measurement systems from the laboratory to the plant is still a real challenge. For example, many processing steps deal with suspensions that lead to plugging and deposition problems. Even if these problems can be handled at the laboratory scale, they still represent formidable challenges at the production level. There is presently a strong push to develop and validate measurement techniques that can work equally well throughout the three levels of Research, Development and Production.

When quality measurements are not directly available, state estimation (or soft sensing) is typically utilized. However, physical on-line measurements are often too unspecific for online state estimation in batch processes (e.g. heat balance models are too insensitive with respect to the chemical transformations of interest). Current practice indicates that there are very few applications of state estimation in specialty chemistry. However, state estimation works well in fermentation processes due to the availability of additional physical measurements and the possibility to reconstruct concentrations without the use of kinetic models (Bastin and Dochain, 1990).

- *Uncertainty:* Uncertainty is widely present in the operation of batch processes. Firstly, it enters in the reactant quality (changes in feedstock), which is the main source of batch-to-batch variations. Secondly, uncertainty comes in the form of modeling errors (errors in model structure and parameters). These modeling errors can be fairly large since, according to the philosophy of batch processing, little time is available for the modeling task. Thirdly, process disturbances and measurement noise contribute to the uncertainty in process evolution (e.g. undetected failure of dosing systems; change in the 'quality' of utilities such as brine temperature, or of manual operations such as solid charge).

  Recipe modifications from one batch to the next to tackle uncertainty are common in the specialty chemical industry, but less so for the exclusive syntheses in agro and pharmaceuticals production. Uncertainty is typically handled through:

  - The choice of conservative operation such as extended reaction time, lower feed rate or temperature, the use of a slightly overstoichiometric mixture in order to force the reaction to fully consume one reactant (Robust mode).
  - Feed stock analyses leading to appropriate adjustments of the recipe (Feedforward mode). Adjustment is usually done by scaling linearly certain variables such as the final time or the dilution, more rarely the feed rate or the temperature.
  - Rigorous quality checks through off-line analyses, or the use of standard measurements such as the temperature difference between jacket and reactor, leading to appropriate correction of the recipe (Feedback mode). For example, a terminal constraint can be met by successive addition of small quantities of feed towards the end of a batch to bring the reaction to the desired degree of completion (Meadows and Rawlings, 1991).

  The problem of scale-up can also be viewed as one of (model) uncertainty. The data available from laboratory studies do not quite extrapolate to the production level. Thus, when the strategies developed in the laboratory are used at the production level, they do carry a fair amount of uncertainty. Furthermore, the pressure to reduce costs and to speed up process development calls for large scale-ups with a considerable amount of extrapolation. As a result, the proposed strategies can be rather conservative.

- *Constraints:* Industrial processing is naturally characterized by soft and hard constraints related to equipment and operational limitations and to safety aspects. In batch processing, there is the additional effect of terminal constraints (selectivity in reaction systems, purity in separation systems, admissible levels of impurities, etc.). Furthermore, in multi-product batch production, the process has to fit in an existing plant. Thus, ensuring feasible operation comes before the issue of optimality, and process designers normally introduce sufficient conservatism in their design so as to guarantee feasibility even in the worst of conditions.

  The need to improve performance calls for a reduction of the conservatism that is introduced to handle uncertainty. Performance improvement can be obtained by operating closer to constraints, which can be achieved by measuring/estimating the process state with respect to these constraints. Riding along an operational constraint is often done when the constrained variable is directly implemented (such as maximum feed rate) or can be measured (such as a temperature).

- *Time-varying decisions:* Traditionally, chemists in the laboratories and operators in the plants were used to thinking in terms of constant values (experimental planning results in static maps between design variables and process performance). New sensors and increasing computing power (e.g. spectroscopic measurements, modern DCS systems) make on-line time-varying decisions possible. Along with these new time-dependent insights, the chemists in the laboratory start to vary process inputs as a function of time. The potential benefit of these additional degrees of freedom is paramount to using optimal control techniques. There are situations where variable input profiles can be of direct interest:
  - There may be a significant theoretical advantage of using a variable profile over the best constant profile (Rippin, 1983). The performance improvement can sometimes be considerable. In batch crystallization, for example, gains of up to 500% can be obtained by adjusting the temperature, the removal of solvent or the addition of a precipitation solvent as functions of time. Large gains are also possible in reactive semi-batch distillation.
  - It is more and more common to adjust the feed rate in semi-batch reactors so as to force the heat generation to match the cooling capacity of the jacket.

An interesting feature of batch processing is the fact that batch processes are repeated over time. Thus, the operation of the current batch can be improved by using the off-line measurements available from previous batches. The objective is then to get to the optimum over as few batches as possible. Also, with the tendency to skip pilot plant investigations whenever possible, this type of process improvement is of considerable interest for the initial batches of a new production campaign.

Implications for Optimization

The industrial situation, as far as technical issues are concerned, can be summarized as follows:

- There is an immediate need to improve the performance of batch processes.
- Models are poor, incomplete or nonexistent.
- On-line measurements are rare, and state estimation is difficult; however, off-line measurements can be made available if needed.
- There is considerable uncertainty (model inaccuracies, variations in feedstock, process disturbances).
- Several operational and safety constraints need to be met.

The implications of the current industrial situation regarding the choice of an appropriate optimization approach are presented in Table 1. The details will be clarified in the forthcoming sections. The main conclusion is that a framework that uses (preferably off-line) measurements rather than a model of the process for implementing the optimal inputs is indeed required.

Industrial situation	Implications for optimization
Need to improve performance	Use optimization for computing time-dependent decisions
Absence of a reliable model	Use measurements for implementing optimal inputs
Few on-line measurements	Use off-line measurements in a batch-to-batch optimization scheme
Presence of uncertainty	Identify and track signals that are invariant to uncertainty
Operational and safety constraints	Track constraints so as to reduce conservatism

Table 1: Implications of the industrial situation regarding the choice of an appropriate optimization approach

Overview of Batch Process Optimization

The optimization of batch processes typically involves both dynamic and static constraints and falls under the class of *dynamic optimization*. Possible scenarios in dynamic optimization are depicted in Figure 1. The first level of classification depends on whether or not uncertainty (e.g., variations in initial conditions, unknown model parameters, or process disturbances) is considered. The standard approach is to discard uncertainty, leading to a nominal solution that may not even be feasible, let alone optimal, in the presence of uncertainty.

The second level concerns the type of information that can be used to combat uncertainty. If measurements are not available, a conservative stand is

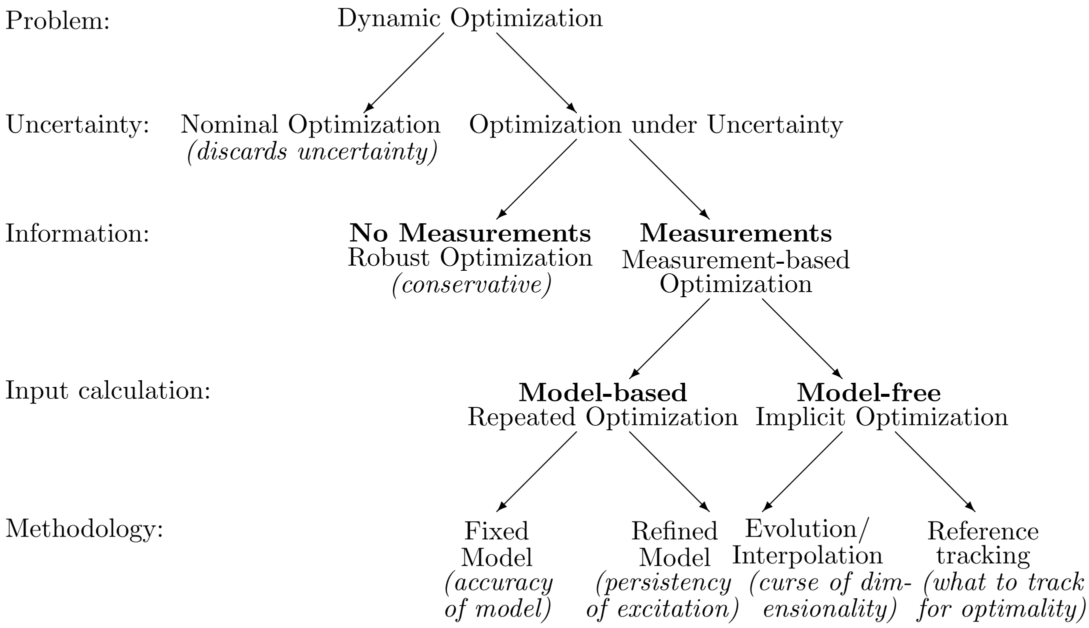

Figure 1: Dynamic optimization scenarios with, in parentheses, the corresponding major disadvantage

required. In contrast, conservatism can be reduced with the use of measurements.

In the next levels, the classification is based on how the measurements are used in order to guide the optimization. The calculation of inputs can be either model-based or model-free. In the model-based case, the type of model that is used (fixed or refined) affects the resulting methodology. If the input calculation is model-free, the current measurement is either compared to a reference or used for interpolation between pre-computed optimal values. The different scenarios are discussed in detail next.

Nominal Optimization

In nominal optimization, the uncertainty is simply discarded. A typical batch optimization problem consists in achieving a desired product quality at the most economical cost, or maximizing the product yield for a given batch time. The optimization can be stated mathematically as follows:

$$\min_{u(t)} J = \phi(x(t_f)) \tag{1}$$

$$s.t. \quad \dot{x} = F(x,u), \quad x(0) = x_0 \tag{2}$$

$$S(x,u) \leq 0, \quad T(x(t_f)) \leq 0 \tag{3}$$

where J is the scalar performance index to be minimized, x the n-vector of states with known initial conditions x_0, u the m-vector of inputs, F a vector field describing the dynamics of the system, S the ζ-vector of path constraints (which include state constraints and input bounds), T the τ-vector of terminal constraints, ϕ a smooth scalar function representing the terminal cost, and t_f the final time.

The problem (1)–(3) is quite general. Even when an integral cost needs to be considered, i.e., $J = \bar{\phi}(x(t_f)) + \int_0^{t_f} L(x,u)dt$, where L a smooth function, it can be converted into the form (1)–(3) by the introduction of an additional state: $\dot{x}_{cost} = L(x,u)$, $x_{cost}(0) = 0$, and $J = \bar{\phi}(x(t_f)) + x_{cost}(t_f) = \phi(x(t_f))$. Let J^* be the optimal solution to (1)–(3). It is interesting to note that the minimum time problem with an additional constraint $\phi(x(t_f)) \leq J^*$, i.e,

$$\min_{t_f, u(t)} \quad t_f \tag{4}$$

$$s.t. \quad \dot{x} = F(x,u), \quad x(0) = x_0 \tag{5}$$

$$S(x,u) \leq 0, \quad T(x(t_f)) \leq 0 \tag{6}$$

$$\phi(x(t_f)) \leq J^* \tag{7}$$

will lead to exactly the same optimal inputs as (1)–(3), though the numerical conditioning of the two problems, (1)–(3) and (4)–(7), may differ considerably. The equivalence of solutions is verified using the necessary conditions of optimality. So, without loss of generality, the final time will be assumed fixed in this paper.

Application of Pontryagin's Maximum Principle (PMP) to (1)–(3) results in the following Hamiltonian (Bryson and Ho, 1975; Kirk, 1970):

$$H = \lambda^T F(x,u) + \mu^T S(x,u) \tag{8}$$

$$\dot{\lambda}^T = -\frac{\partial H}{\partial x}, \quad \lambda^T(t_f) = \left.\frac{\partial \phi}{\partial x}\right|_{t_f} + \nu^T \left.\left(\frac{\partial T}{\partial x}\right)\right|_{t_f} \tag{9}$$

where $\lambda(t) \neq 0$ is the n-vector of adjoint states (Lagrange multipliers for the system equations), $\mu(t) \geq 0$ the ζ-vector of Lagrange multipliers for the path constraints, and $\nu \geq 0$ the τ-vector of Lagrange multipliers for the terminal constraints. The Lagrange multipliers μ and ν are nonzero when the corresponding constraints are active and zero otherwise so that $\mu^T S(x,u) = 0$ and $\nu^T T(x(t_f)) = 0$ always. The first-order necessary condition for optimality of the input u_i is:

$$H_{u_i} = \frac{\partial H}{\partial u_i} = \lambda^T \frac{\partial F}{\partial u_i} + \mu^T \frac{\partial S}{\partial u_i} = \lambda^T F_{u_i} + \mu^T S_{u_i} = 0. \tag{10}$$

Note that, in this paper, PMP will not be used to determine the optimal solution numerically since this procedure is well known to be ill-conditioned (Bryson, 1999). However, PMP will be used to decipher the characteristics of the optimal solution.

Robust Optimization

In the presence of uncertainty, the classical *open-loop* implementation of off-line calculated nominal optimal inputs may not lead to optimal performance. Moreover, constraint satisfaction, which becomes important in the presence of safety constraints, may not be guaranteed unless a conservative strategy is adopted. In general, it can be assumed that the model structure is known and the uncertainty concentrated in the model parameters and disturbances. Thus, in the uncertain scenario, the optimization can be formulated as follows:

$$\begin{aligned} \min_{u(t)} J &= \phi(x(t_f)) \\ s.t. \quad & \dot{x} = F(x,\theta,u) + d, \quad x(0) = x_0 \\ & S(x,u) \leq 0, \quad T(x(t_f)) \leq 0 \end{aligned} \tag{11}$$

where θ is the vector of uncertain parameters, and $d(t)$ the unknown disturbance vector. In addition, the initial conditions x_0 could also be uncertain.

To solve this optimization problem, an approach referred to as *robust optimization*, where the uncertainty is taken into account explicitly, is proposed in the literature (Terwiesch et al., 1994). The uncertainty is dealt with by considering all (several) possible values for the uncertain parameters. The optimization is performed either by considering the worst-case scenario or in an expected sense. The solution obtained is conservative but corresponds to the *best* possibility when measurements are not used.

Measurement-based Optimization (MBO)

The conservatism described in the subsection above can be considerably reduced with the use of measurements, thereby leading to a better cost. Consider the optimization problem in the presence of uncertainty and measurements as described below:

$$\begin{aligned} \min_{u^k_{[t_l,t_f]}} J^k &= \phi(x^k(t_f)) \\ s.t. \quad & \dot{x}^k = F(x^k,\theta,u^k) + d^k, \; x^k(0) = x^k_0 \\ & y^k = h(x^k,\theta) + v^k \\ & S(x^k,u) \leq 0, \; T(x^k(t_f)) \leq 0 \\ \text{given} \quad & y^j(i), \; i = \{1,\cdots,N\} \\ & \forall \, j = \{1,\cdots,k-1\}, \text{ and} \\ & i = \{1,\cdots,l\} \text{ for } j = k. \end{aligned} \tag{12}$$

where $x^k(t)$ is the state vector, $u^k(t)$ the input vector, $d^k(t)$ the process disturbance, $v^k(t)$ the measurement noise, and J^k the cost function for the k^{th} batch. Let $y = h(x,\theta)$, a p-dimensional vector, be the combination of states that can be measured, $y^j(i)$ the i^{th} measurement taken during the j^{th} batch, and N the number of measurements within a batch. The objective is to utilize the measurements from the previous $(k-1)$ batches and the measurements up to the current time, t_l, of the k^{th} batch in order to tackle the uncertainty in θ and determine the optimal input policy for the remaining time interval $[t_l, t_f]$ of the k^{th} batch.

Role of the model in the calculation of the inputs. Among the measurement-based optimization schemes, a classification can be done according to whether or not a model is used to guide the optimization.

Model-based input calculation: Repeated optimization. In optimization, the model of the system can be used to predict the evolution of the system, compute the cost sensitivity with respect to input variations so as to obtain search directions, and update the inputs towards the optimum. Measurements are then used to estimate the current states and parameters. As the estimation and optimization tasks are typically repeated over time, this scheme is often referred to as repeated optimization. The model is either fixed or refined using measurements, the advantages and disadvantages of which are discussed next.

- *Fixed model*: If the model is not adjusted, it needs to be fairly accurate. This, however, is against the philosophy of the approach that assumes the presence of (considerable) uncertainty. If the uncertainty is only in the form of disturbances and not in the model parameters, it might be sufficient to use a fixed model. On the other hand, if the model is not accurate enough, the methodology will have difficulty converging to the optimal solution. Note that, since the measurements are used to estimate the states only (and not the parameters), there is no need for persistent inputs.
- *Refined model*: When model refinement is used, the need to start with an accurate model is alleviated, but it is necessary to excite appropriately the system for estimating the uncertain parameters. However, the optimal inputs may not provide sufficient excitation. On the other hand, if sufficiently exciting inputs are provided for parameter identification, the resulting solution may not be optimal. This leads to a conflict between the objectives of parameter estimation and optimization. This conflict has been studied in the adaptive control literature under the label *dual control problem* (Roberts and Williams, 1981; Wittenmark, 1995).

Model-free input calculation: Implicit optimization. In this approach, measurements are used directly to update the inputs towards the optimum, i.e., without using a model and explicit numerical optimization. However, a model might be used *a priori* to characterize the optimal solution. The classification here is based on whether the measurement is used for interpolation between pre-computed optimal values or simply compared to a reference.

- *Evolution/interpolation*: The inputs are computed from past data and current measurements. If only batch-end measurements are used, the difference in cost between successive experimental runs can be used to provide the update direction for the inputs (evolutionary programming). The on-line version of this approach is based on the feedback optimal solution – the solution to the Hamilton-Jacobi-Bellman equation (Kirk, 1970) – being stored in one form or the other (e.g., neural network, look-up table, or dynamic programming).

  The main drawback of this approach is the curse of dimensionality. A large number of experimental runs are needed to converge to the optimum if only batch-end measurements are used. The use of the method with on-line measurements requires either a computationally expensive look-up table or a closed-form feedback law, which is analytically expensive or impossible to obtain in many cases.
- *Reference tracking*: The inputs are computed using feedback controllers that track appropriate references. The main question here is what references should be tracked. In most of the studies found in the literature, the references correspond to optimal trajectories computed off-line using a nominal model. Such an approach, however, is not guaranteed to be optimal in the presence of uncertainty. As will be explained later, this paper uses the concept of invariants to chose references, the tracking of which implies optimality.

Type of measurements. The type of measurements (off-line or on-line) can add another level to the classification of optimization strategies.

- *Off-line measurements:* Off-line measurements include measurements taken at the end of the batch (batch-end measurements) and, possibly, off-line analysis of samples taken during the batch. These measurements cannot be used to improve the current batch but only subsequent ones. Off-line measurements are most common in industrial practice. They enable the set-up of a *batch-to-batch optimization* approach to account for parametric uncertainty by exploiting the fact that batch processes are typically repeated. Process knowledge obtained from previous batches is used to update the operating strategy of the current batch. This approach requires solving an optimization problem at the beginning of each batch. The objective is then to get to the optimum over a few batches.
- *On-line measurements:* When information is available during the course of the batch, an *on-line optimization* approach can be used. Measurements are used to compensate for uncertainty both within the batch and, possibly, also in a batch-to-batch manner. With this compensation, the variability caused by uncertainty is reduced to a large extent. Thus, it is possible

to guarantee feasibility with smaller conservative margins which, in turn, helps improve the cost.

MBO *vs.* **MPC**. Model-predictive control (MPC), which has been well studied in the literature (see Rawlings et al. (1994); Qin and Badgwell (1997); Morari and Lee (1999) for surveys), has both some overlap and differences with MBO schemes that form the subject of this paper. MPC typically uses the repeated optimization approach to solve a control problem in an optimal manner. The major points that distinguish MBO from MPC are discussed next.

- *Goal and cost function:* The goal in MPC is control – choose the inputs to track given references – whereas the goal in MBO is optimization – maximize the yield of a product, minimize time for a given productivity, etc. In MPC, the control problem is formulated as an optimization with the cost function reflecting the quality of control, which typically is quadratic in nature, i.e., $J = \int_0^{t_f} \left(x^T Q\, x + u^T R\, u\right)\, dt$. In contrast, the cost function in MBO reflects the economic objective to optimize. However, once the optimization problem is formulated, similar tools are used for solution.
- *Continuous vs. batch processes:* MPC is oriented principally towards continuous processes. Stability is the main issue there and has been studied extensively in the MPC literature (Mayne et al., 2000). In contrast, MBO is oriented towards batch processes with a finite terminal time. Stability does not play a crucial role, and there is even a tendency to destabilize the system towards the end for the sake of optimality (the so-called batch kick). The important issues in MBO are feasibility and feedback optimality – how optimal is the operation in the presence of constraints and uncertainty. In contrast to MPC, MBO schemes can take advantage of the fact that batches are typically repeated. Run-to-run and implicit optimization schemes are thus particular to the MBO literature.
- *Role of constraints:* MBO typically has solutions that are on the constraints since the potential of optimization arises mainly from the presence of path and terminal constraints. Thus, it is important to go as close to the constraints as possible and, at the same time, guarantee feasibility. In contrast, though MPC has been designed to handle constraints, the typical problems considered in the framework of MPC try to avoid the solution being on the constraints by introducing a compromise between tracking performance and input effort.

Certain MBO schemes in the category of repeated optimization have been referred to as MPC schemes in the literature (Eaton and Rawlings, 1990; Meadows and Rawlings, 1991; Helbig et al., 1998; Lakshmanan and Arkun, 1999) and, thus, fall in the grey area between Batch MPC (Lee et al., 1999; Chin et al., 2000) and MBO for batch processes. It might be interesting to note that the search for optimality *via* tracking has also been studied for continuous processes. The terms "self-optimizing control", "feedback control", or "constraint control" are often used. The reader is referred to (Skogestad, 2000) for an overview of the work done in this area.

Classification of measurement-based optimization methods. Only MBO methods (as opposed to MPC methods) that have been designed to deal explicitly with uncertainty in batch processing are considered in the classification. Table 2 illustrates the interplay between the type of measurements (off-line vs. on-line) and the role played by the model (model-based vs. model-free adaptation). Representative studies available in the literature are placed in the table.

Invariant-based Optimization

The idea of Invariant-Based Optimization (IBO) is to identify those important characteristics of the optimal solution that are invariant under uncertainty and provide them as references to a feedback control scheme. Thus, optimality is achieved by tracking these references without repeating numerical optimization. Also, the fact that batches are typically repeated over time can be used advantageously, thereby providing the possibility of on-line and/or batch-to-batch implementation. The methodology consists of:

1. a parsimonious state-dependent parameterization of the inputs,
2. the choice of signals that are invariant under uncertainty, and
3. the tracking of invariants using measurements.

These three steps are discussed in the following subsections.

Methodology	Batch-to-batch optimization (Off-line measurements)	On-line optimization (On-line measurements)
Model-based Fixed model	Zafiriou and Zhu (1990) Zafiriou et al. (1995) Dong et al. (1996)	Meadows and Rawlings (1991) Agarwal (1997) Abel et al. (2000)
Model-based Refined model	Filippi-Bossy et al. (1989) Marchal-Brassely et al. (1992) Rastogi et al. (1992) Fotopoulos et al. (1994) Le Lann et al. (1998) Ge et al. (2000) Martinez (2000)	Eaton and Rawlings (1990) Ruppen et al. (1998) Gattu and Zafiriou (1999) Noda et al. (2000) Lee et al. (2000)
Model-free Evolution Interpolation	Clarke-Pringle and MacGregor (1998)	Tsen et al. (1996) Rahman and Palanki (1996) Yabuki and MacGregor (1997) Krothapally et al. (1999) Schenker and Agarwal (2000)
Model-free Reference tracking	Scheid et al. (1999) Srinivasan et al. (2001)	Soroush and Kravaris (1992) Terwiesch and Agarwal (1994) Van Impe and Bastin (1995) Saenz de Buruaga et al. (1997) Ubrich et al. (1999) Fournier et al. (1999) Gentric et al. (1999) Lakshmanan and Arkun (1999) Visser et al. (2000)

Table 2: MBO methods specifically designed to compensate uncertainty

Piecewise Analytic Characterization of the Optimal Solution

The parsimonious state-dependent parameterization arises from intrinsic characteristics of the optimal solution. The optimal solution is seen to possess the following properties (Visser et al., 2000):

- The inputs are in general discontinuous, but are analytic in between discontinuities. The time at which an input switches from one interval to another is called a *switching time*.
- Two types of arcs (constraint-seeking and compromise-seeking) are possible between switching instants. In a constraint-seeking arc, the input is determined by a path constraint, while in the other type of interval, the input lies in the interior of the feasible region (Palanki et al., 1993). The set of possible arcs is generically labelled $\eta(t)$.

The structure of the optimal solution is described by the type and sequence of arcs which can be obtained in three ways:

- educated guess by an experienced operator,
- piecewise analytical expressions for the optimal inputs,
- inspection of the solution obtained from numerical optimization.

In the most common third case, a simplified model of the process is used to compute a numerical solution in which the various arcs need to be identified. The exercise of obtaining the analytical expressions for the optimal inputs is undertaken only if the numerical solution cannot be interpreted easily. This analysis is, in general, quite involved and is only intended to provide insight into what constitutes the optimal solution rather than to implement the optimal solution. This analysis is discussed next.

Constraint-seeking *vs.* compromise-seeking arcs.

Constraint-seeking arc for u_i (Bryson and Ho, 1975). In this case, the input u_i is determined by an active constraint, say, $S_j(x,u) = 0$. Thus, $\mu_j \neq 0$. If $S_j(x,u)$ depends explicitly on u_i (e.g., in the case of input bounds), the computation of the optimal u_i is immediate. Otherwise, since $S_j(x,u) = 0$ over the entire interval under consideration, its time derivatives are also zero, $\frac{d^k}{dt^k} S_j(x,u) = 0$, for all k. Note that the time differentiation of $S_j(x,u)$ contains $\dot{x}$, i.e., the dynamics of the system. $S_j(x,u)$ can be differentiated with respect to time until u_i appears. The optimal input is computed from that time derivative of $S_j(x,u)$ where u_i appears. The computed input u_i is typically a function of the states of the system, thus providing a feedback law.

Compromise-seeking arc for u_i (Palanki et al., 1993). In this arc, none of the path constraints pertaining to the input u_i is active. The input is then determined from the necessary condition of optimality, i.e., $H_{u_i} = \lambda^T F_{u_i} = 0$. If F_{u_i} depends explicitly on u_i, the computation of the optimal u_i is immediate. Otherwise, since $H_{u_i} = 0$ over the entire interval, the time derivatives of H_{u_i} are also zero, $\frac{d^k}{dt^k} H_{u_i} = 0$, for all k. H_{u_i} can be differentiated with respect to time until u_i appears, from which the optimal input is computed. The computed input is a function of the states and might possibly also depend on the adjoint variables. If u_i does not appear at all in the time differentiations of H_{u_i}, then either no compromise-seeking arcs exist or the optimal input u_i is non-unique (Baumann, 1998).

The fact that the optimal inputs are in the interior of the feasible region is the mathematical representation of the physical tradeoffs present in the system and affecting the cost. If there is no intrinsic tradeoff, the input u_i does not appear in the successive time differentiations of H_{u_i}. This forms an important subclass for practical applications. It guarantees that the optimal solution is always on the path constraints. This is the case in controllable linear systems, feedback-linearizable systems, flat systems, and involutive-accessible systems, a category which encompasses many practical systems (Palanki et al., 1993; Benthack, 1997).

Constraint-seeking *vs.* compromise-seeking parameters.

Parsimonious input parameterization. The pieces described above are sequenced in an appropriate manner to obtain the optimal solution. The switching times and, possibly, a few variables that approximate the compromise-seeking arcs completely parameterize the inputs. The decision variables of the parameterization are labelled π. In comparison with piecewise constant or piecewise polynomial approximations, the parameterization proposed is exact and parsimonious.

Optimal choice of π. Once the inputs have been parameterized as $u(\pi, x, t)$, the optimization problem (1)–(3) can be written as:

$$\min_{\pi} J = \phi(x(t_f)) \quad (13)$$

$$s.t. \quad \dot{x} = F(x, u(\pi, x, t)), \; x(0) = x_0 \quad (14)$$

$$T(x(t_f)) \leq 0 \quad (15)$$

Some of the parameters in π are determined by active terminal constraints (termed the *constraint-seeking parameters*) and some from sensitivities (termed the *compromise-seeking parameters*). Note the similarity with the classification of arcs for input u_i. Without loss of generality, let all τ terminal constraints be active at the optimum. Consequently, the number of decision variables arising from the parsimonious parameterization, n_π, needs to be larger than or equal to τ in order to satisfy all terminal constraints.

The idea is then to separate those variations in π that keep the terminal constraints active from those that do not affect the terminal constraints. For this, a transformation $\pi^T \rightarrow [\bar{\pi}^T \; \tilde{\pi}^T]$ is sought such that $\bar{\pi}$ is a τ-vector and $\tilde{\pi}$ a $(n_\pi - \tau)$-vector with $\frac{\partial T}{\partial \tilde{\pi}} = 0$. A linear transformation which satisfies these properties can always be found in the neighborhood of the optimum. Then, the necessary conditions for optimality of (13)–(15) are:

$$T = 0, \quad \frac{\partial \phi}{\partial \bar{\pi}} + \nu^T \frac{\partial T}{\partial \bar{\pi}} = 0, \quad \text{and} \quad \frac{\partial \phi}{\partial \tilde{\pi}} = 0. \quad (16)$$

The active constraints $T = 0$ determine the τ decision variables $\bar{\pi}$ while $\tilde{\pi}$ are determined from the sensitivities $\frac{\partial \phi}{\partial \tilde{\pi}} = 0$. Thus, $\bar{\pi}$ corresponds to the constraint-seeking parameters and $\tilde{\pi}$ to the compromise-seeking parameters. The Lagrange multipliers ν are calculated from $\frac{\partial \phi}{\partial \bar{\pi}} + \nu^T \frac{\partial T}{\partial \bar{\pi}} = 0$.

Signals Invariant under Uncertainty

In the presence of uncertainty, the numerical values of the optimal input u_i in the various arcs and the input parameters π might change considerably. However, what remains invariant under uncertainty is the fact that the necessary condition $H_{u_i} = 0$ has to be verified. $H_{u_i} = 0$ takes on different expressions for constraint-seeking and compromise-seeking arcs. To ease the development, it is assumed that the uncertainty is such that it does not affect the type and sequence of arcs nor the set of active terminal constraints.

Choice of invariants.

Choice of invariants for constraint-seeking and compromise-seeking arcs. A set of signals $I_i^\eta(t) = h_i^\eta(x(t), u(t), t)$, referred to as *invariants* for arcs, will be chosen such that optimality is achieved by tracking $I_{ref,i}^\eta = 0$. Note the dependence of h_i^η with respect to t, which indicates that h_i^η can be different in different intervals of the optimal solution.

Tracking $H_{u_i} = 0$ has different interpretations with respect to the two types of arcs. In the case of a constraint-seeking arc for u_i with the constraint S_j being active, $H_{u_i} = \lambda^T F_{u_i} + \mu_j \frac{\partial S_j}{\partial u_i} = 0$, with $\mu_j \neq 0$ and $\lambda^T F_{u_i} \neq 0$. The constraint has to be active for the sake of optimality since otherwise μ_j is zero and $H_{u_i} \neq 0$. Thus, the invariant along a constraint-seeking arc is $h_i^\eta(x, u, t) = S_j(x, u)$. For a compromise-seeking arc, $H_{u_i} = \lambda^T F_{u_i} = 0$. Therefore, the invariant is $h_i^\eta(x, u, t) = \lambda^T F_{u_i}(x, u)$.

Note that the element that remains invariant despite uncertainty is the fact that optimal operation corresponds to $I_{ref}^\eta = 0$. However, the uncertainty does have an influence on the value of $I^\eta(t)$, and the inputs need to be adapted in order to guarantee $I_{ref}^\eta = 0$.

Choice of invariants for constraint-seeking and compromise-seeking parameters. In addition to the choice of invariants for the various arcs, it is important to choose the invariants for the parameters π. Following similar arguments, a set of signals $I^\pi = h^\pi(x(t_f))$ can be constructed such that the optimum corresponds to $I_{ref}^\pi = 0$, also in the presence of uncertainty. Clearly, the invariants arise from the conditions of optimality. For the constraint-seeking parameters, they correspond to the terminal constraints $h^\pi(x(t_f)) = T(x(t_f))$ and, for the compromise-seeking parameters, to sensitivities $h^\pi(x(t_f)) = \frac{\partial \phi(x(t_f))}{\partial \tilde{\pi}}$.

To summarize, the invariants are as follows:

- For constraint-seeking arcs:
  $h_i^\eta(x, u, t) = S_j(x, u)$
- For compromise-seeking arcs:
  $h_i^\eta(x, u, t) = \lambda^T F_{u_i}(x, u)$
- For constraint-seeking parameters:
  $h^\pi(x(t_f)) = T(x(t_f))$
- For compromise-seeking parameters:
  $h^\pi(x(t_f)) = \frac{\partial \phi(x(t_f))}{\partial \tilde{\pi}}$

Sensitivity of the cost. The sensitivity of the cost to non-optimal operation is in general much lower along a compromise-seeking arc than along a constraint-seeking arc. Consider the optimal input u_i determined by the path constraint S_j and the optimality condition $H_{u_i} = \lambda^T F_{u_i} + \mu_j \frac{\partial S_j}{\partial u_i} = 0$ with $\mu_j \neq 0$. If the input does not keep the constraint active, μ_j becomes zero. Thus, the change in cost is directly proportional to $\lambda^T F_{u_i}$, which is non-zero. In contrast, along a compromise-seeking arc, $H_{u_i} = \lambda^T F_{u_i} = 0$, and a small deviation of u_i from the optimal trajectory will result in a negligible loss in cost. Similarly, as seen from (16), the deviation in cost arising from the non-satisfaction of a terminal constraint is proportional to $\nu^T \frac{\partial T}{\partial \tilde{\pi}}$, whilst a small variation of $\tilde{\pi}$ cause negligible loss in cost.

In summary, it is far more important to track the path constraints S_j than the sensitivity $\lambda^T F_{u_i}$. Furthermore, it is far more important to track the terminal constraints T than the sensitivities $\frac{\partial \phi}{\partial \tilde{\pi}}$. Consequently, it is often sufficient in practical situations to focus attention only on constraint-seeking arcs and parameters.

Tracking of Invariants

The core idea of the optimization scheme is to use a model to determine the structure of the optimal inputs and measurements to update a few input parameters and the value of the inputs in some of the intervals. This way, the optimal inputs are determined directly from process measurements and not from a (possibly inaccurate) model.

Optimality despite uncertainty is approached by working close to the active constraints, i.e., where there is much to gain! Indeed, tracking path and terminal constraints is usually much more important than regulating sensitivities as was argued above. The structure given in Figure 2 is proposed to track the invariants by use of feedback (Srinivasan et al., 1997; Visser, 1999; Visser et al., 2000). The two major blocks are described below:

- *Analysis:* This level consists of a simplified (not necessarily accurate) model of the process. The tasks are as follows:

  1. The numerical optimizer solves the optimization problem using the simplified model and provides the nominal signals x^* and u^*.
  2. The type and sequence of arcs are deci-

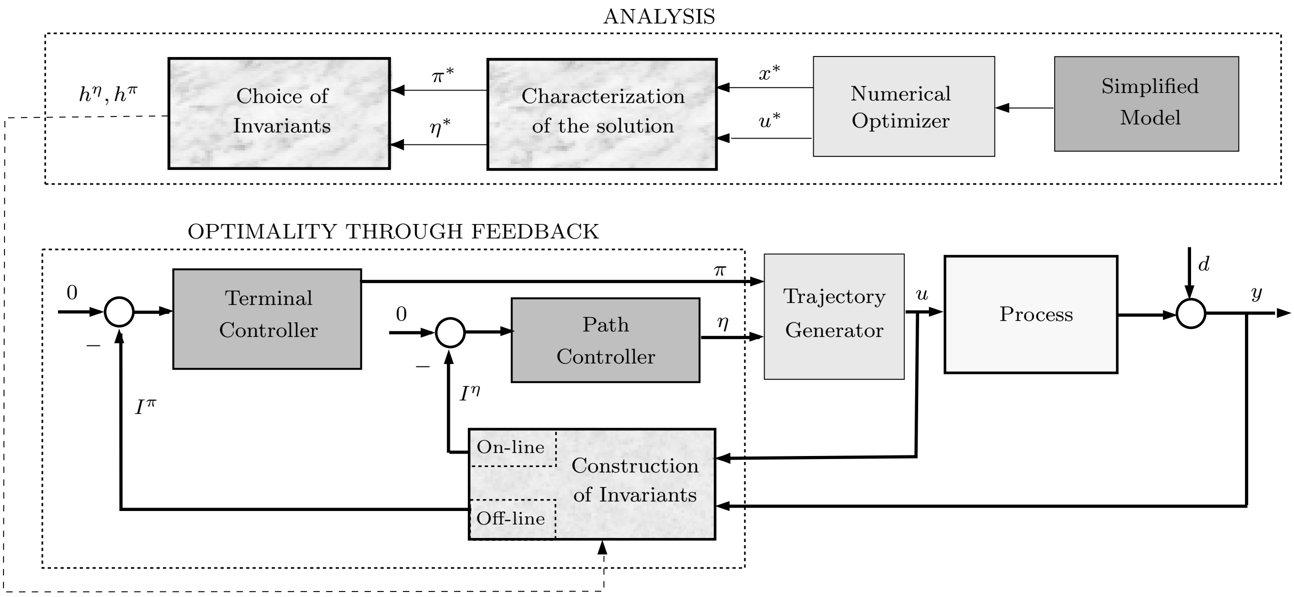

Figure 2: Invariant-based optimization

phered from the numerical solution, leading to a parsimonious parameterization of the inputs (characterization of the optimal solution).

3. The invariant functions $h^\eta(x(t), u(t), t)$ and $h^\pi(x(t_f))$ are obtained as proposed earlier. Note that the switching strategy is inherent in the choice of h^η.

- *Optimality through feedback:* The invariants $I^\eta_{ref} = 0$ and $I^\pi_{ref} = 0$ are tracked with the help of path and terminal feedback controllers, respectively. The trajectory generator computes the current inputs as a function of $\eta(t)$ and π.

The model-based 'Analysis' is normally carried out off-line once, and only the measurement-based 'Optimality through feedback' operates on-line during process runs. Thus, the implementation is *model-free* and *measurement-based.*

Practical applicability of IBO

If the model and the true (unknown) system share the same input structure (type and sequence of arcs) and the same active terminal constraints, IBO will be capable of optimizing the true system. Thus, the value of IBO in practice will depend on both the robustness of the proposed input structure with respect to uncertainty (modeling errors and disturbances) and the ability to measure the path and terminal constraints. These issues are briefly discussed next.

- *Role of the model.* Although the implementation of optimal inputs in the invariant-based scheme is truly model-free, a model may still be needed at the analysis step. The role of the model is to determine the structure of the optimal inputs, i.e., the type and the sequence of arcs and the set of active constraints. The structure of the inputs is obtained either numerically or *via* educated guesses, with the proposed input structure being verified using PMP necessary conditions on the nominal model. The approach is directly applicable to large-scale industrial process, as long as the nominal model and the real system share the same input structure. So, in contrast to model-based approaches or what is sought of for simulation purposes, there is no need for a detailed model or for accurate parameter values. The model simply needs to reflect the major tradeoffs specific to the optimization problem at hand. The parts of the model that do not address these effects can be discarded.
- *Construction of invariants from measurements.* Since I^η and I^π are not measured directly, they need to be reconstructed from the available measurements. In the case of constraint-

seeking arcs and parameters, the invariants correspond to physical quantities (path or terminal constraints). Off-line measurements of terminal quantities are in general available. On-line measurements to meet path constraints might be more difficult. Three cases can be considered:

1. The path constraint deals directly with a physical quantity that can be easily measured such as temperature or pressure.
2. The path constraint deals with a quantity that cannot be directly measured, but the constraint can be rewritten with respect to something that can be measured. This is, for example, possible when a heat removal constraint can be rewritten as a constraint on a cooling temperature.
3. Cases 1 and 2 do not apply, and some type of inference or state estimation is necessary to meet the constraint. This case is clearly more involved than the two preceding ones. The reconstruction problem is closely related to inferential control (Joseph and Brosilow, 1978; Doyle, 1998). However, it may well happen that a conservative approach for meeting the path constraint (requiring easily-available or no measurements) is sufficient.

On the other hand, for compromise-seeking arcs and parameters, the invariants are sensitivities. For computation of sensitivities, either a model of the process or multiple process runs are required, which is typically more difficult. However, as discussed above, the sensitivity with respect to input variations in compromise-seeking arcs and parameters can often be neglected. In such a case, all compromise-seeking arcs and parameters are kept at their off-line determined values, and only the constraint-seeking arcs and parameters are adjusted.

- *Difference in time scale – on-line vs. off-line measurements.* In general, there is a difference in time scale between the path controller and the terminal controller. The path controller works within a batch using on-line measurements (running index is the batch time t) (Benthack, 1997). The terminal controller operates on a batch-to-batch basis using off-line measurements (running index is the batch number k) (Srinivasan et al., 2001).

  If on-line measurements are not available, the path controller is inactive. If off-line measurements of the path constraint are available, it is possible to use the path controller in a batch-to-batch mode so that the system will be closer to the path constraint during the next batch (Moore, 1993). On the other hand, if it is possible to predict I^π from on-line measurements, it might be possible to use the terminal controller within the batch (Yabuki and MacGregor, 1997).

  The presence of disturbances influences both $\eta(t)$ and π. Disturbances affecting $\eta(t)$ within the batch are rejected by the path controller. However, the effect of any disturbance within the batch on π cannot be rejected since the terminal controller only works on a batch-to-batch basis. Constant disturbances (e.g. raw material variations) can be rejected from batch-to-batch by the terminal controller.

- *Backoff from constraints.* In the presence of disturbances and parametric uncertainty that cannot be compensated for by feedback, the use of conservative margins, called backoffs, is inevitable to ensure feasibility of the optimization problem (Visser et al., 2000). The presence of measurement errors also necessitates a backoff. Based on an estimate of the uncertainty, the probability density function of the state variables can be calculated. The margins are then chosen such that the spread of the states remains within the feasible region with a certain confidence level. Note that the margins typically vary with time.
- *Reduction of backoff.* Due to the sensitivity reduction characteristic of feedback control, the conservatism can be reduced considerably in the proposed framework in comparison with the standard open-loop optimization schemes. The feedback parameters can be chosen so as to minimize the spread in the state variables resulting from uncertainty. The use of feedback becomes particularly important when the uncertainty tends to increase during a batch run. With reduced backoffs, the process can be driven closer to active constraints, thereby leading to improved performance.

Example - Semi-batch Reactor with Safety and Selectivity Constraints

Description of the Reaction System

- *Reaction:* $A + B \rightarrow C$, $2\ B \rightarrow D$.
- *Conditions:* Semi-batch, isothermal.

- *Objective:* Maximize the amount of C at a given final time.
- *Manipulated variable:* Feed rate of B.
- *Constraints:* Input bounds; limitation on the heat removal rate through the jacket; constraint on the amount of D produced.
- *Comments:* The reactor is kept isothermal by (say) adjusting the cooling temperature in the jacket, T_c. B is fed at the temperature $T_{in} = T$. To remain isothermal, the power generated by the reactions, q_{rx}, must be evacuated through the cooling jacket, i.e., $q_{rx} = UA(T - T_c)$. Thus, the heat removal constraint can be expressed in terms of a lower bound for the cooling temperature, T_{cmin}. The variables and parameters are described in the next subsection.
  Without any constraints, optimal operation would consist of adding the available B at initial time (i.e., batch mode). The presence of the heat removal constraints calls for semi-batch operation with constraint-seeking arcs. Furthermore, the constraint on the amount of D that can be produced imposes a compromise-seeking feeding of B in order to maximize C without violating the terminal constraint on D.

Problem Formulation

Variables and parameters: c_X: Concentration of species X, n_X: Number of moles of species X, V: Reactor volume, u: Feed rate of B, c_{Bin}: Inlet concentration of B, k_1, k_2: Kinetic parameters, ΔH_1, ΔH_2: Reaction enthalpies, T: Reactor temperature, T_c: Cooling temperature in the jacket, T_{in}: Feed temperature, U: Heat transfer coefficient, A: Surface for heat transfer, and q_{rx}: power produced by the reactions. The numerical values are given in Table 3.

Model equations:

$$\dot{c_A} = -k_1 c_A c_B - \frac{u}{V} c_A \quad (17)$$

$$\dot{c_B} = -k_1 c_A c_B - 2\,k_2 c_B^2 + \frac{u}{V}(c_{Bin} - c_B) \quad (18)$$

$$\dot{V} = u \quad (19)$$

with the initial conditions $c_A(0) = c_{Ao}$, $c_B(0) = c_{Bo}$, and $V = V_o$. Assuming $c_C(0) = c_D(0) = 0$, the concentration of the species C and D are given by $c_C = \frac{c_{Ao}V_o - c_A V}{V}$ and $c_D = \frac{(c_{Bo}V_o - c_B V) + c_{Bin}(V - V_o) - (c_{Ao}V_o - c_A V)}{2\,V}$. The power produced by the reactions and T_c are given by

$$q_{rx} = k_1\ c_A\ c_B(-\Delta H_1)V + 2\ k_2\ c_B^2(-\Delta H_2)V \quad (20)$$

$$T_c = T - \frac{q_{rx}}{U\,A} \quad (21)$$

Optimization problem:

$$\begin{aligned} \max_{u(t)} \quad & J = n_C(t_f) \qquad (22) \\ s.t. \quad & (17) - (19) \\ & T_c(t) \geq T_{cmin} \\ & n_D(t_f) \leq n_{Df_{max}} \\ & u_{min} \leq u \leq u_{max} \end{aligned}$$

k_1	0.75	l/(mol h)
k_2	0.014	l/(mol h)
ΔH_1	-7×10^4	J/mol
ΔH_2	-5×10^4	J/mol
c_{Bin}	10	mol/l
UA	8×10^5	J/Kh

u_{min}	0	l/h
u_{max}	100	l/h
T_{cmin}	10	°C
$n_{Df_{max}}$	5	mol

c_{Ao}	2	mol/l
c_{Bo}	0	mol/l
V_o	500	l
t_f	2.5	h

Table 3: Model parameters, operating bounds and initial conditions

Piecewise Analytic Characterization

Using Pontryagin's Maximum Principle, it can be shown that the competition between the two reactions results in a feed that reflects the optimal compromise between producing C and D. This compromise-seeking input can be calculated from the second time derivative of H_u as:

$$u_{comp} = \frac{V\,c_B(k_1 c_A(2\,c_{Bin} - c_B) + 4\,k_2 c_B c_{Bin})}{2\,c_{Bin}\,(c_{Bin} - c_B)} \quad (23)$$

The other possible arcs correspond to the input being determined by the constraints: (i) $u = u_{min}$, (ii) $u = u_{max}$, and (iii) $u = u_{path}$. The input u_{path} corresponds to riding along the path constraint $T_c = T_{cmin}$. The input is obtained by differentiating the path constraint once with respect to time, i.e., from $\dot{T_c} = 0$:

$$\begin{aligned} u_{path} &= \left.\frac{\mathcal{N}}{\mathcal{D}}\right|_{T_c = T_{cmin}} \qquad (24) \\ \mathcal{N} &= c_B V\Big(\Delta H_1 k_1 c_A(k_1(c_A + c_B) + 2\,k_2 c_B) \\ &\quad + 4\,\Delta H_2 k_2 c_B(k_1 c_A + 2\,k_2 c_B)\Big) \end{aligned}$$

$$\mathcal{D} = \Delta H_1 k_1 c_A (c_{Bin} - c_B) + 4\,\Delta H_2 k_2 c_B (2\,c_{Bin} - c_B)$$

Sequence of arcs and parsimonious parameterization:

- The input is initially at the upper bound, $u = u_{max}$, in order to attain the path constraint as quickly as possible.
- Once T_c reaches T_{cmin}, $u = u_{path}$ is applied in order to keep $T_c = T_{cmin}$.
- The input switches to $u = u_{comp}$ at the time instant π so as to take advantage of the optimal compromise in order to maximize $n_c(t_f)$ and meet the terminal constraint $n_D(t_f) = n_{Df_{max}}$.

Since analytical expressions for the input in the various arcs exist, the optimal solution can be parameterized using only the switching time between the path constraint and the compromise-seeking arc. This parameter π is determined numerically so as to satisfy the terminal constraint $n_D(t_f) = n_{Df_{max}}$. The invariants I^η correspond to the input bound in the first interval, the path constraint in the second interval and the sensitivity $\lambda^T F_u$ for the compromise-seeking arc. For the switching time, the invariant is the terminal constraint itself. The optimal input is shown in Figure 3 with the optimal values $\pi = 1.31\,h$ and $J = 600.6$ mol.

Note that the input u_{path} given by (24) will keep the system on the path constraint once the path constraint $T_c = T_{cmin}$ is attained, but will not keep the path constraint active in the presence of uncertainty. The same can be said for u_{comp} in (23). Thus, the analytical expressions for u_{path} and u_{comp} will only be used for interpretation of the nominal optimal trajectory and not for implementation of the true optimal solution. At the implementation level, simple PI-controllers will be used.

Measurement-based Optimization

In practice, there can be considerable uncertainty both in the stoichiometric and kinetic models. This is reflected here as some uncertainty for the kinetic parameter k_1 in the interval $0.4 \leq k_1 \leq 1.2$ (The nominal value $k_1 = 0.75$ used in the simulation is assumed to be unknown). In order not to violate the constraints, a conservative feed profile (Figure 3) would have to be designed so that: i) the path constraint is not violated for $k_1 = k_{1max} = 1.2$,

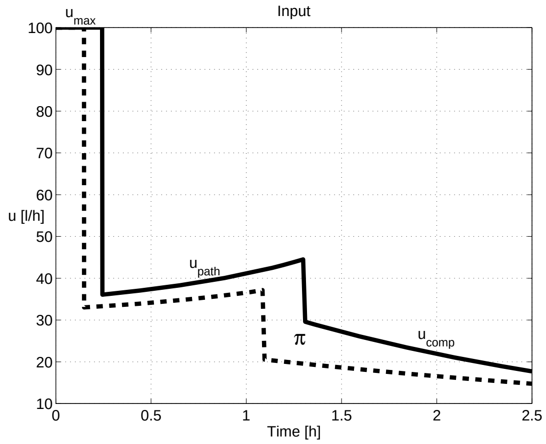

Figure 3: Nominal optimal input (solid) and Conservative optimal input (dotted)

and ii) the terminal constraint is not violated for $k_1 = k_{1min} = 0.4$ (a small k_1 corresponds to more B in the reactor and thus to a higher production of D). So, the conservative profile would consist of computing u_{path} and the first switching instant using $k_1 = k_{1max}$, and adjusting π so that the terminal constraint is satisfied for $k_1 = k_{1min}$.

With respect to the measurements available, different optimization scenarios are considered:

1. *No measurements:* The conservative optimal feed profile defined above is applied open loop to the simulated nominal plant.
2. *Batch-end measurements:* Only the measurement of $n_D(t_f)$ is available and, thus, the switching time π is updated in a batch-to-batch manner. For the second interval, $u_{path} = u_{path}^{cons}$, the conservative value computed off-line using k_{1max} is applied. Due to the low sensitivity of the cost with respect to the fine shape of the input in the compromise-seeking interval, the latter is approximated by the constant value $u_{comp} = 20$ (l/h).
3. *On-line and batch-end measurements:* On-line measurement of the cooling jacket temperature T_c is available. The path constraint is kept active using the feedback $u_{path}(t) = u_{path}^{cons} + k_p\,(T_{cmin} - T_c(t)) + k_i \int_0^t (T_{cmin} - T_c(t))dt$, where k_p and k_i are the parameters of a PI controller. In addition, the switching time π is updated in a batch-to-batch manner. As in Scenario 2, the compromise-seeking arc is approximated by $u_{comp} = 20$ (l/h).

The cases of both noise-free and noisy measurements

	Optimization Scenario	Terminal Constraint $n_D(t_f)$ mol ($n_{Df_{max}} = 5$ mol)	Path Constraint $\min_t T_c(t)$ ^oC ($T_{c,min} = 10^oC$)	Cost (mol)	Loss
1	Open-loop application of optimal conservative input	2.71	12.87	498.8	20%
2	Adaptation of π using off-line measurements (with 5% noise)	4.75	11.62	582.6	3%
	Adaptation of π using off-line measurements (no noise)	5.00	11.50	589.2	2%
3	Adaptation of $u_{path}(t)$ and π using on-line and off-line measurements (with 5% noise)	4.75	11.25	590.9	1.5%
	Adaptation of $u_{path}(t)$ and π using on-line and off-line measurements (no noise)	5.00	10.00	600.5	0.02%

Table 4: Invariant-based optimization. Results averaged over 100 noise realizations, each consisting of run-to-run adaptation over 50 batches.

(5% relative Gaussian measurement noise) are considered. The results are given in Table 4. If the measurements are noisy, a conservative margin (backoff) needs to be incorporated so as to guarantee feasibility. The backoffs are 0.25 mol for $n_{Df_{max}}$ and 1.25^{o}C for T_{cmin}.

It is seen that with only off-line (or batch-end) measurements, the terminal constraint can be satisfied by adapting the switching instant π. The evolutions of the switching instant and the cost for batch-to-batch optimization are shown in Figures 4 and 5. It can be seen that the solution gets close to the optimum within a few batches.

If, in addition, on-line measurements are available, the path constraint can be kept active as well. Thus, it is possible to get very close to the optimum by using measurements. The loss of 0.02% in the last noise-free scenario is due to the approximation of the compromise-seeking arc by the constant value $u_{comp} = 20$ (l/h).

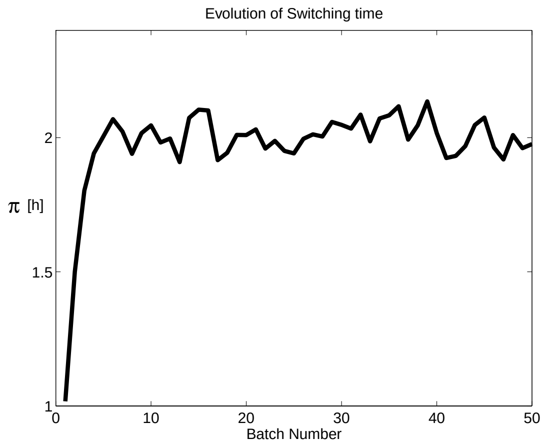

Figure 4: Evolution of switching time for one realization of the batch-to-batch optimization with only batch-end measurements (5% measurement noise)

Discussion

The model was only necessary to obtain the type and sequence of arcs: u_{max}, u_{path} and u_{comp}. As far as the implementation is concerned, $u_{max} = 100$ l/h is part of the problem formulation, u_{path} is determined by a PI-controller upon tracking T_{cmin}, and $u_{comp} = 20$ l/h is a constant-value approximation to the optimal profile computed off-line using the model. The switching time π between u_{path} and u_{comp} is adjusted in a run-to-run manner by a PI-controller in order to meet $n_{Df_{max}}$. The actual value of u_{comp} is of little relevance as any error in u_{comp} can be easily compensated for by an appropriate shift in π.

Assume that, in addition to the two modeled reactions, the true system also includes $B + C \rightarrow E$,

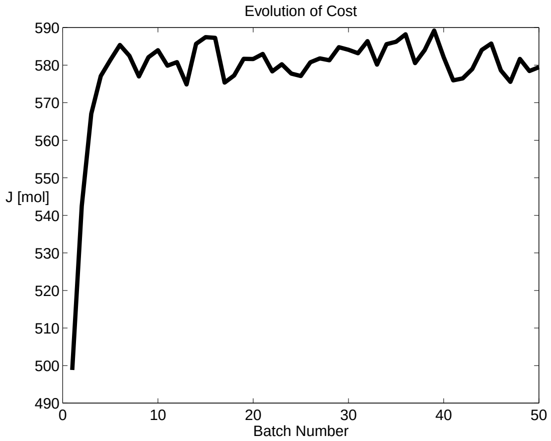

Figure 5: Evolution of cost for the same scenario as in Figure 4

$B \rightarrow F$. This would not affect the type and sequence of arcs since the two additional reactions are similar to the second reaction with respect to the effect of the input u, i.e., they consume B away from the first (desired) reaction. Thus the proposed scheme would be equally applicable even in the presence of the two additional reactions.

In the formulation of the optimization problem it was assumed $T_{in} = T$. Even without this assumption, the proposed approach is applicable. The possibility of removing heat through temperature increase of the feed from T_{in} to T (so-called sensible heat) changes the heat removal constraint to:

$$q_{rx} - q_{in} \leq UA(T - T_{cmin}) \tag{25}$$

with q_{in} the rate of heat removal due to the feed of B. However, the implementation of the heat removal constraint remains unchanged as it concerns only the RHS of (25): $u_{path}(t)$ is determined as the output of a PI-controller designed to track T_{cmin}.

A final important remark: The model parameters given in Table 3 are not used for calculating the optimal feed rate. Only the off-line measurement of $n_D(t_f)$ and the on-line measurement of $T_c(t)$ are used to implement the proposed optimizing scheme.

Conclusions

This paper has addressed several optimization issues that directly affect the operation of batch processes. It is argued that process improvement is necessary for the economic well-being of many batch manufacturers. The industrial practice specific to the batch specialty chemistry is presented, with an emphasis on both organizational and technical problems. On the organizational side, the lack of global thinking in dealing with the individual steps of a complex process limits the potential for performance improvement. On the technical side, important limitations regarding both modeling and measurement aspects impair the use of optimization techniques. In addition, batch processes are characterized by a considerable amount of uncertainty and the presence of operational and safety constraints.

The lack of reliable models, together with the presence of uncertainty, has favored the investigation of process improvement *via* utilization of measurements (sometimes on-line, most often off-line). This paper has classified measurement-based optimization methods reported in the literature according to whether or not a model is used to guide the optimization and the type of measurements (on-line, off-line) available.

The major contribution towards process improvement of a constrained batch process is through operation on active constraints. Thus, a feedback-based framework has been proposed to keep the system 'close' to the active constraints. If only off-line measurements are available, this framework results in a batch-to batch optimization scheme with the objective to meet the terminal constraints within a few batches. If on-line measurements are available, the path constraints can also be kept active.

The proposed invariant-based optimization scheme addresses most of the requirements stemming from industrial practice and needs that were listed in Table 1. More specifically,

- it is aimed at process improvement via the use of time-dependent inputs,
- it is model-independent as far as implementation is concerned,
- if necessary, it uses only available off-line measurements,
- it is robust against uncertainty since signals that are invariant under uncertainty are tracked, and finally,
- it guarantees feasibility since the constraints are approached from the safe side.

The approach proposed is effective when the optimization potential stems mainly from meeting path and/or terminal constraints. Such is the case in most of the batch process optimization problems.

It is possible to perceive the proposed feedback-based optimization strategy from an industrial perspective. Classical PID control is the most popular technique used currently in industry, and trading it to attain optimality is unacceptable industrially. Therefore, in contrast to most model-based optimization studies, this work attempts to use feedback control for the sake of optimality. In this sense, the approach has great industrial potential and could help take optimization to the batch chemical industry.

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