Speech at IFAC2014

Thank you Professor Craig for the introduction. IFAC President, distinguished guests, conference organizers, sponsors, colleagues, friends; Good evening

It is indeed fitting to start by thanking the IFAC President, Professor Ian Craig, for inviting me to be part of this gathering. I am honored and privileged to be here.

BACKGROUND

When I was initially invited to speak, my first reaction was an unequivocal no, simply because Automatic Control is largely at the periphery of what I would call my forte. As a principle, I tend not to pronounce on matters that I do not sufficiently understand. After giving the request some thought, I realised that I was actually wrong.

I work in Integration of Batch Chemical Processes; Multipurpose Batch Chemical Processes, to be more specific. These operations have become very common in recent times due to their flexibility and adaptability to variations in demand and quality; a situation mostly encountered in pharmaceutical and speciality chemical industries. Batch chemical processes are broadly categorized into multiproduct and multipurpose batch plants. In multiproduct batch plants, each produced batch follows the same sequence of unit operations from raw materials to final products. However, the produced batch need not belong to the same product and the duration of tasks corresponding to different products can vary.

Consequently, multiproduct batch facilities are ideally suited to products with identical and fixed recipes. If the recipes of the products involved vary from one batch to another, multipurpose batch facilities, tend to be the ideal choice. The variation in recipes for the different batches does not necessarily mean the variation in products. In other words, the same product can have different recipes. As a result, multipurpose batch facilities are appropriate in the manufacture of products that are characterized by variations in recipes.

It is evident from the foregoing description that multipurpose batch chemical plants are combinatorially more complex than multiproduct batch plants. This complexity is not only confined to operation of the plant, but also extends to mathematical formulations that describe multipurpose batch plants. Invariably, a mathematical formulation that describes multipurpose batch plants is also applicable to multiproduct batch plants. However, the opposite is not true. It is solely for this reason that most of the effort in the development of mathematical models for batch chemical plants should be aimed at multipurpose rather than multiproduct batch plants.

Batch Chemical Process Integration is a specialized branch of the broader field of Process Integration. As you may all know, Process Integration is not necessarily a new field; it was founded in the late 70's for energy optimization and evolved to what became known as Pinch Technology, with most contributions emanating from the then University of Manchester Institute of Science and Technology, my alma mater. Implicitly, the technology was geared towards continuous processes at steady-state. It has been applied with great success ever since, not only in energy optimization, but also in resource conservation. However, there is always an aspect of this success that is rarely reported in literature. Steady-state, which is very close to the heart of every chemical engineer, does not actually exist – certainly not by itself. At the very best, it is only with the aid of advanced control systems that steady-state can be realized. Consequently, it is automatic control that is behind the success of Pinch Technology. That observation implies that there exists a confluence between process integration and automatic control. So, I belong to this family.

PROCESS INTEGRATION IN BATCH PROCESSES

But let me hasten to qualify that relationship. Batch processes are fundamentally distinct from continuous processes, in the sense that, even with the most advanced of control systems a batch process will never attain steady-state. These operations are inherently dynamic. The implication, therefore, is that any technique or mathematical model developed for a continuous process cannot be directly applied to batch plants. This distinction is also true for control systems. A control system that is well suited to continuous processes would require prior adaptation before application to batch processes. This is just the tip of the iceberg.

The unique complexities that characterize multipurpose batch plants deserve a dedicated mention here. In the main these pertain to *Time*, *Intrinsic Uncertainties*, *Operational Philosophies* and *Nonlinearities.*

Time

In understanding the implications of time, we should accept the definition of a batch process as that which has to follow a predefined sequence of discrete tasks from raw materials to final products. In reality, it is the *discreteness* of tasks that differentiates batch processes from their continuous counterparts. The discreteness of tasks implies that time is distributed throughout the process and cannot be frozen. Consequently, it is paramount that time is addressed in an almost exact manner in describing batch chemical processes. Any attempt that seeks to bypass or override this fundamental feature of batch processes is likely to fail at worst and be too inaccurate at best. Capturing the essence of time, commonly known as scheduling, is arguably one of the most challenging aspects of batch chemical process integration.

In published literature there exist 3 types of methods in which the influence of time is handled. The first type involves the use of time average models (TAMs) which ultimately treat batch plants as pseudo-continuous operations. As aforementioned this cannot yield results that are a true representation of reality insofar as it attempts to describe batch processes. The second type treats time as a fixed parameter that is known *a priori* with no opportunity for change within the time horizon of interest. The main drawback of this approach is that true optima associated with treating time as a variable rather than a parameter are likely to be overlooked. The traditional graphical targeting techniques on which process integration is founded are highly amenable to these 2 types of methods, since they treat time as a suppressed dimension in the analysis. This consequently allows the analysis to be confined to 2 dimensions, which is an inherent feature of most graphical techniques. The third type of methods treats time in an exact manner by allowing it to vary in search of a true optimum.

Needless to mention, the exact capturing of time presents further challenges in the analysis. Fundamentally, a decision has to be made on how the time horizon has to be represented. Early methods relied on even discretization of the time horizon, although there are still methods published to date that still employ this concept. The first drawback of even time discretization is that it inherently results in a significant binary dimension, particularly when the granularity of the problem is too small compared to the time horizon of interest. The fact that the scheduling problem is a proven NP-Hard Problem suggests that an increase in binary variables renders the problem unsolvable in polynomial time. The second drawback is that, in unit operations where time is likely to vary with the amount of material processed, this technique is not readily usable. A typical example here is distillation.

Recent approaches tend to adopt the continuous-time representation of the time horizon of interest wherein each time point along the time horizon coincides with either the start or the end of a task. In addition to accurate representation of time this approach results in a much smaller binary dimension. The significant drawback here is that the optimal number of time points has to be determined *a priori*, which involves a lengthy iterative process before solving the actual problem. Secondly, almost invariably, the sequence constraints are characterized by the Big-M formulation, which is a structural disadvantage. However, the Big-M in this formulation is deterministic and sufficiently tight, since it is always the time horizon of interest.

Perhaps I should mention at this stage that, slightly more than a week ago we had a visit from two of the leading experts in this area at Wits University in Johannesburg, Professors Ignacio Grossmann and Larry Biegler from Carnegie Mellon University in Pittsbugh, USA. They tell me that some of the recent formulations using even discretization of the time horizon have outperformed the continuous-time formulations, which is the strongest sign to date that the even discretization of the time horizon could structurally superior to continuous-time, regardless of the number of binary variables.

Uncertainty

Whilst all chemical processes entail an element of uncertainly due to unavoidable variations in raw materials, which have a direct influence in processing times, batch processes, in particular, entail a strong human intervention factor. This further compounds the aspect of uncertainty. The human intervention factor is, in most instances, a consequence of limited automatic control.

Operational philosophies

As a way of debottlenecking the process, batch operations make significant use of intermediate storage or buffer tanks. These are either shared among various tasks within the process or dedicated to each stage. The use of storage is also dependent on the stability of intermediates. Unstable intermediates have to be processed immediately after formation, implying a near-zero residence time in storage. In the case of stable intermediates, the capacity of storage becomes a major constraint that has to be built into the model. Overall, there are at least six different operational philosophies.

Nonlinearity of constraints

In modeling batch chemical processes, nonlinearities emanate from component material balances and reaction kinetics. In most instances the component balances can be linearized exactly, in the case of bilinear terms that entail at least one binary variable or inexactly, where bilinear terms involve only continuous variables. Linearization of the latter commonly makes use of over and underestimators, which generally yield reasonable convergence if the bounds are fairly tight. Glover transformation remains unrivaled as an exact linearization technique where binary variables are involved. Most of the reaction kinetics could be convexified without losing nonlinearity if global optimality is the main goal.

AUTOMATED CONTROL IN BATCH CHEMICAL PLANTS

The problem that I have just described in sufficient detail, assumes some static set of conditions, like fixed mixing ratios and task duration times. In other words, it is a highly simplified problem, although it is still largely unsolvable. Otherwise, it would have been an ideal platform on which to build automatic control logic of practical relevance. Any control logic that is based on a deterministic schedule cannot handle the intrinsic complexities of the dynamic and agile environment.

THE CONCLUSION

In conclusion, the problem that is yet to be solved is the one involving scheduling and process control within a comprehensive framework. If it is indeed true that time, hence the schedule, is the core of any batch chemical process, then the optimality of synthesis and design of current operations remains questionable. In essence, we have a living example of an animal vaccine facility, not too far from here, which we have proven to be 70% overdesigned using mathematical tools.

Thank you