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Towards the systematic design of actuation for process systems

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Abstract: Currently systematic design of actuation (operational degrees of freedom) for process systems is not possible because (i) the required domain knowledge has not been identified and (ii) it is unclear how to explore the relation between actuation and operational improvement. This paper proposes geometry and flux equations as the required domain knowledge. It is explained that the relation between actuation and operational improvement should be explored in an optimal control setting. By means of an example (distillation) it is illustrated that a spatial actuation extension may result in considerable operational improvement.

Keywords: Systematic design, actuation, process systems, operation mode, optimal control.

1. INTRODUCTION

Generally speaking actuation, the presence of operational Degrees Of Freedom [1] (DOF) enables the manipulation of system behavior. More specifically in the case of process systems actuation allows to:

(1) Keep the process within the operational envelope even though there is uncertainty.
(2) Achieve the product quantity and quality targets as required by the market.
(3) Improve operational performance in a technological or even economic sense.

The first two points deal with constraining process variables, so these points are directly related to controllability. The last point boils down to optimization.

How is actuation designed? In order to answer that question it is has to be understood that actuation is really a part of Conceptual Process Design (CPD) since it has an impact on one or more balances. This can easily be illustrated by means of an example. Consider the continuous stirred tank reactor shown in figure 1, left. In the reactor an exothermic reaction takes place. By adding a cooling mantle and a control valve in the cooling water line, heat transfer is actuated and this allows for the temperature to be controlled (see figure 1, right).

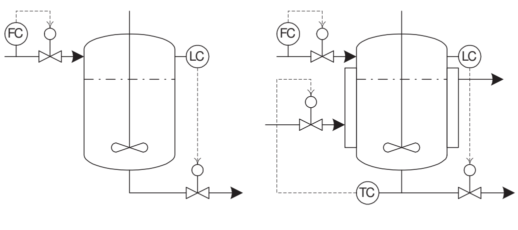

Fig. 1. Actuation of a continuous stirred tank reactor.

[1] Also known as control DOF, manipulated variables, manipulative variables, input variables or inputs.

The heat balance for both situations is clearly different. Note that sensing is not a part of the CPD; for example adding a temperature sensor to the reactor does not change the heat balance. Sensing is handled in the detailed engineering. According to Douglas (1988) the CPD is done after selecting the operation mode (batch or continuous). Lewin (1999) points out that the control design takes place after the process design. So the overall conceptual design consists of three stages (see figure 2).

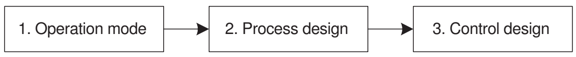

Fig. 2. The three stages of overall conceptual design.

Roozenburg and Eekels (1995) explain that the various activities that take place during design are described by the so-called basis cycle of design (see figure 3). Although Roozenburg and Eekels (1995) discuss the cycle in the context of industrial design it can also be found in process design Siirola (1996) and mechanical design Cross (1994). The cycle is in fact a tailored form of the scientific method for design problems.

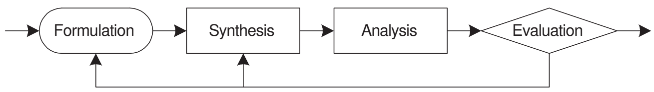

Fig. 3. The four phases of the basis cycle of design.

In the formulation phase the basis of design is defined. This means specification of required performance, relevant external factors, selection of the design space including building blocks and identification of the required domain knowledge. Next in the synthesis phase alternatives are generated. The behavior of the proposed alternatives is determined in the analysis phase. And finally in the evaluation phase the performance of the alternatives is compared with the specified performance as defined in the formulation phase. If the performance is not acceptable the synthesis or even formulation phase should be revisited.

We will now analyze CPD and especially the current practice of actuation design by means of the basis cycle of design:

Formulation The basis of design of CPD boils down to: Given a certain operation mode and external factors come up with a process design that is feasible, safe, economically attractive and environmentally acceptable. Actuation is related to feasibility more specifically i/o controllability. Typical external factors are type of feed, the availability of utilities, ambient temperature range and so on. For actuation disturbances are the most important external factor. The building blocks for CPD are unit operations and they also span the design space. The knowledge on unit operations constitutes a major part of the domain knowledge. It is tempting to say that actuators are the building blocks for actuation and that the type of actuators (control valve, variable speed drive, etc.) span the design space. But does this mean that the domain knowledge for actuation is just related to actuators? The answer must be no since "there is a gap between an actuator and having an impact on one or more balances". *It seems that there is a lack of domain knowledge on actuation.* This invites the question: What is known in the literature about actuation? This question will be answered later.

Synthesis Normally at least a few alternative CPD's are generated. These alternatives differ in reactor type, distillation sequence etc., so they differ with respect to the type and order of unit operations. It should be noted that actuation alternatives are not synthesized explicitly by the process engineer. So differences in actuation between the alternatives are "coincidental" rather than systematic. This situation is probably not a matter of focus but the logical result of the already perceived lack of domain knowledge on actuation.

Analysis This phase deals with simulation but also with economic estimations. Actuation can be included by means of controllability calculations. All calculations are normally done in a short-cut way. For example in the case of continuous operation simulation is done by a static flowsheeter while controllability calculations are based on indices (relative gain array, minimum singular value, relative disturbance gain etc.).

Evaluation All alternatives are compared with the basis of design. Typically a ranking takes place with respect to feasibility (this can include controllability), safety, economics and environmental performance. It should be noted that the CPD only reveals the impact of actuation on controllability. *The possible influence of actuation on improving operational performance remains invisible.* This is mainly a direct consequence of fixing the operation mode before the CPD (what is fixed can not be improved).

We will now return to the question: What is known in the literature about actuation? The contributions fall in two categories. The first category has to do with determining the number of DOF. Ponton (1994), Pham (1994) and Konda et al. (2006) provide alternatives for the "#variables minus #equations" approach which requires a detailed model, is time consuming and error sensitive. The second category connects process design or input selection with controllability. Fisher et al. (1988) explain that for an uncontrollable process design controllability can be restored by (i) adding more manipulative variables, (ii) overdesign of certain equipment and (iii) ignoring optimization of the least important operating variables. The authors give a few examples of (i): "add bypasses, add purge streams, add auxilliary condensers and reboilers" yet no systematic method is offered. Skogestad and Postlethwaite (1996) describe how an uncontrollable acid neutralization process (single tank with base injection) becomes controllable by a process design change (two tanks in series with separate base injection). However the authors don't explain the background of the design modification. An overview of i/o selection methods is presented by van de Wal and de Jager (2001). But the authors do not elaborate how a complete list of inputs can be obtained. Furthermore they define i/o selection as decisions on the number, location and type of actuators and sensors. As stated before actuation involves changes in the CPD, so actuation is not just a matter of placing a number of a certain type of actuators.

The discussion up till now shows that systematic design of actuation for process systems is not possible because of two outstanding questions:

(1) What is the domain knowledge needed to understand actuation of process systems?
(2) How can the relation between actuation and operational improvement be explored?

We will try to answer both questions. The rest of this paper is organized as follows. Section 2 focuses on the first question. Section 3 proposes a systematic method for generating actuation alternatives and discusses two options for restoring controllability. Section 4 compares the concept of operation mode with an optimal control setting as possibilities to explore the relation between actuation and operational improvement. Section 5 illustrates by means of an example (distillation) that a spatial actuation extension may result in considerable operational improvement. The last section summarizes the conclusions and provides suggestions for further work.

2. ACTUATION DOMAIN KNOWLEDGE

It was already mentioned that actuation enables the manipulation of system behavior. In the case of mechanical systems it is quite intuitive that actuation implies exerting force. However actuation of process systems is not a trivial issue; what is the process equivalent of applying force?

In this paper a process is defined as a system that converts material and/or energy [2]. In process systems four phenomena play an important role:

(1) Chemical reaction.
(2) Transfer of mass.
(3) Transfer of heat.
(4) Transfer of momentum.

All these phenomena involve fluxes [3] and geometry (volume or area). Combining this with the general viewpoint leads to: Actuation implies manipulation of fluxes and/or

[2] Energy conversion should be associated by material conversion but material conversion should not involve transmutation.
[3] In the case of chemical reaction, flux is also referred to as rate.

geometry. Fluxes are the result of deviations from thermodynamic equilibrium. These deviations can be expressed as so-called driving forces. The relation between fluxes and driving forces is given by flux equations. From irreversible thermodynamics it is known that all flux equations contain a phenomenological coefficient and a driving force. This means that in principle each phenomena can be manipulated in three ways:

- By coefficient; for example mixing jets in fluidized beds manipulate the heat transfer coefficient.
- By driving force; for example reaction rates are often manipulated via the reactant concentration.
- By geometry; for example in flooded condensers the available heat exchange area is manipulated.

However often the coefficient is determined by material properties and/or flow conditions while the geometry is fixed during the process design. This then leaves only the option of actuation by driving force. By now it is probably clear that the role force plays in mechanical systems is fulfilled by driving force in process systems. It is worth noting that in the well known balance equation "accumulation = in - out + production - conversion" all right hand side terms are in fact fluxes integrated over the relevant geometry.

3. GENERATING ACTUATION ALTERNATIVES

The essential point of the previous section is the insight: *Actuation implies manipulation of fluxes and/or geometry.* This insight allows to generate actuation alternatives in a systematic way:

(1) Make a list of all the phenomena involved. The "list of four phenomena" serves as a starting point.
(2) Select the phenomena that should be actuated. Consider the addition of extra fluxes.
(3) Write down the flux equations of the selected phenomena. Indicate the relevant geometry.
(4) Analyze the flux equations for the three actuation options; coefficient, driving force and geometry.

In the case of distributed systems fluxes can be place dependent. This opens the possibility of spatial actuation. However with the exception of reactors spatial actuation is not used much in process systems; most distributed systems are only actuated at one or both ends of the system. The authors of this paper believe that especially spatial actuation of process systems deserves more attention.

It was already mentioned that according to Fisher et al. (1988) controllability can be restored by (i) adding more manipulative variables, (ii) overdesign of certain equipment and (iii) ignoring optimization of the least important operating variables. The last option basically means accepting the situation as it is; not an attractive option. We will now compare option (i) and (ii) by means of an example. Consider a mixing process (figure 4, left).

In a mixer a large flow F_{in} is mixed with a small flow containing an additive F_{ad}. The objective is to keep the concentration of additive C in the outlet flow F_{out} at a fixed value regardless of fluctuations in F_{in}. For good mixing a certain minimal volume V is required, it is

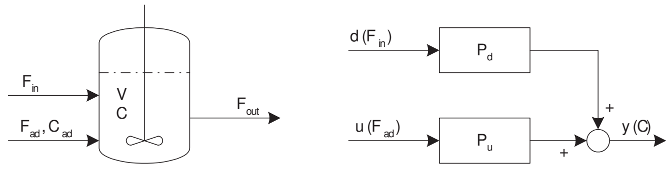

Fig. 4. A mixing process; the flow scheme (left) and the block diagram (right).

assumed that this volume is sufficient and constant. The dynamic model for this process boils down to a total mass balance and a mass balance for the additive. The block diagram obtained after linearization is shown in figure 4, right. The two transfer functions are given by:

$$P_d = \frac{K_d}{\tau s + 1} \quad (1)$$

$$P_u = \frac{K_u}{\tau s + 1} \quad (2)$$

Suppose that the control is done by proportional feedback control with a gain K_c. Then disturbance rejection and setpoint tracking are given by:

$$\frac{y(s)}{d(s)} = \frac{K_d}{\tau s + 1 + K_u K_c} \quad (3)$$

$$\frac{y(s)}{r(s)} = \frac{K_u K_c}{\tau s + 1 + K_u K_c} \quad (4)$$

Here r is the setpoint and s the Laplace variable. For the base case the following values are taken: $K_u = 1$, $K_d = 1$, $K_c = 1$ and $\tau = 10$. In order to improve the closed-loop performance two possibilities are investigated:

- A design modification; the mixer volume is increased by a factor 10. Since $\tau = V/(F_{in} + F_{ad})$, this implies that τ increases to 100.
- An actuation modification; the range is increased by a factor 10. Since this is the only limiting factor for pole placement K_c can be increased to 10.

The resulting bode plots (amplitude ratio only) of the sensitivity and complementary sensitivity functions are shown in figure 5.

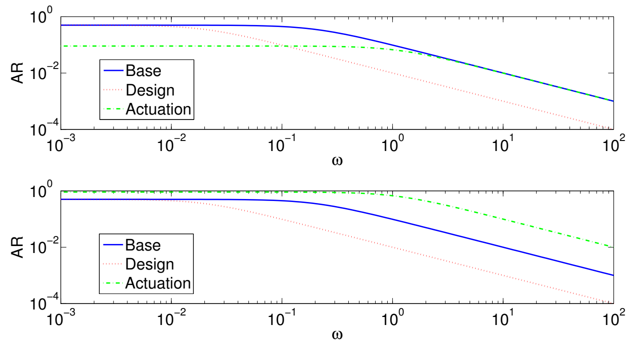

Fig. 5. The amplitude ratio of the sensitivity (above) and complementary sensitivity (below) functions.

It is clear that the design and actuation modification both improve disturbance rejection. However this is not true for setpoint tracking; only the actuation modification gives a better performance, the design modification actually leads to a worse performance. The explanation is straightforward, a larger volume helps to filter disturbances but also means a more sluggish response when changing the operating point. For actuation this trade-off between regulator and servo behavior simply does not exist, it improves both.

So controllability can indeed be restored by actuation as well as overdesign. However overdesign just improves regulator behavior at the expense of servo behavior. Actuation improves regulator as well as servo behavior. Furthermore overdesign will be a more expensive and less safe option than actuation since it directly translates in larger equipment size and increased intermediate storage. *The conclusion is that restoring controlllability is preferably done by actuation.* It is not difficult to grasp that this conclusion will hold in general for process systems.

4. IMPROVING OPERATIONAL PERFORMANCE

As explained in the introduction the CPD is proceeded by the selection of an operation mode. There seems to be general agreement that at least four operation modes can be recognized:

(1) Continuous; feed and product flow from and to the environment in a continuous way. All bulk chemicals are produced in this way.
(2) Batch; feed and product flow from and to the environment in a discontinuous way. This mode is used for most specialty chemicals.
(3) Fed-batch; as batch but the feed is introduced during (a part of) the batch. This mode is relevant for biochemical processes.
(4) Periodic; the process is manipulated deliberately in a periodic way. This mode is used for example in flow reversal reactors.

The typical trajectories are shown in figure 6.

Only continuous operation can lead to a stationary situation (all internal process variables become constant over time). In the case of (fed-)batch operation accumulation of product takes place while periodic operation is deliberately non-stationary. It can be argued that more operation modes exist. For example a distillation column under total reflux is operated in a completely “closed” mode since there is no feed and product flow from and to the environment.

The choice for a particular mode is based on heuristics. And there are only heuristics available to guide the decision: Batch or continuous operation? Table 1 presents some of these heuristics, for more information see Douglas (1988) and Smith (1995). The idea behind table 1 is to estimate which mode is technically feasible and economically attractive.

Table 1. Continuous versus batch operation.

	Batch	Continuous
Production rate	$< 1 * 10^6$ lb/yr	$> 10 * 10^6$ lb/yr
Flexibility	multi product	single product
Reaction time	no limitation	typically < 30 min.

Basically the use of a mode means that process operation is based on a class of trajectories. However process operation can also be based on an optimal control problem. Huesman et al. (2008) have formulated economic optimal operation as:

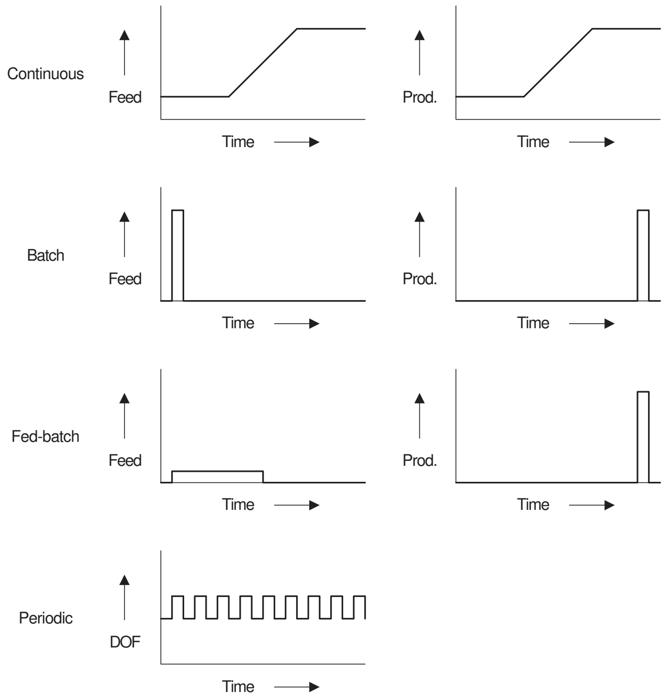

Fig. 6. The trajectories for the various operation modes.

$$\max \int_0^{t_f} \text{Profit.dt} \quad \text{s.t.} \begin{cases} \text{plant dynamics} \\ \text{operational limitations} \\ \text{scheduling constraints} \end{cases} \tag{5}$$

Here t_f stands for the time horizon. The authors explain that if the revenues are fixed the objective simplifies to the minimization of cost. An obvious question is now: What kind of operation (mode) results from such a formulation? Two general comments can be made:

- Huesman et al. (2008) show that the solution can be non-unique. Consider the following optimal control problem:

$$\min \sum_{k=1}^{25} u_k \quad \text{s.t.} \begin{cases} 0 \leq u_k \leq 5 \\ x_{k+1} = x_k + 0.25u_k \\ x_1 = 0 \\ x_{25} = 2.5 \end{cases} \tag{6}$$

Two possible solutions are shown in figure 7.

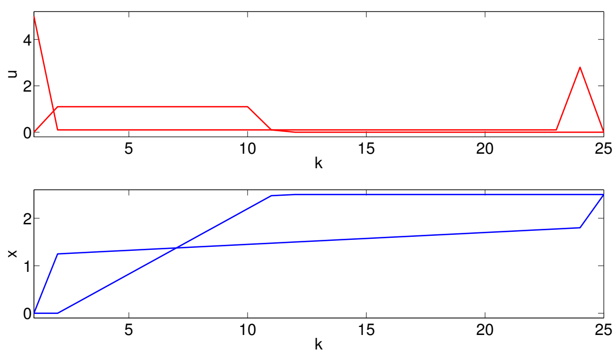

Fig. 7. The solution of optimal control problem (6).

However there are in fact an infinite number of solutions. Basically this means that an economic objective does not necessarily fix all degrees of freedom and lexicographic optimization should be considered. Similar results were found by van Essen et al. (2009) for economic optimization of oil production from petroleum reservoirs. It seems that the presence of integrators in the plant dynamics plays an important role in the occurrence of non-unique solutions.

- Rawlings and Amrit (2009) point out that in the case of a convex objective, a sufficient long time horizon and linear plant dynamics the optimal dynamic solution will converge to the optimal stationary solution (the so-called turnpike theorem). Consider the following optimal control problem:

$$\max \sum_{k=1}^{25} 5x_k - 2u_k \quad \text{s.t.} \begin{cases} 0 \le u_k \le 5 \\ x_{k+1} = 0.5x_k + 0.25u_k \\ x_1 = 0 \text{ or } 4 \end{cases} \quad (7)$$

The two unique solutions are shown in figure 8.

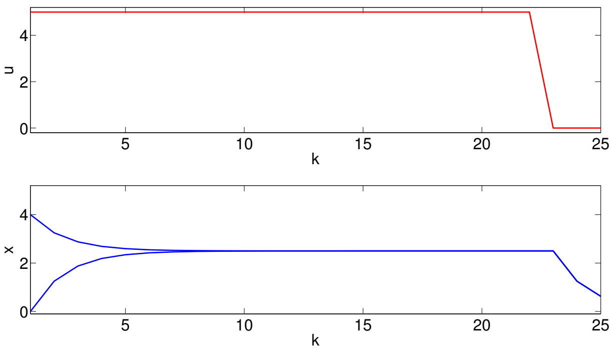

Fig. 8. The solution of optimal control problem (7).

Note that regardless of the initial condition the solution converges to $u = 5$ and $x = 2.5$; the optimal stationary solution. Of course plant dynamics are typically non-linear and this may lead for instance to periodic solutions.

Process operation based on operation mode is seriously limited by the concept of a fixed mode, the small number of modes (classes do not overlap) and the heuristics that are used to choose a particular mode. On the other hand process operation based on optimal control is only limited by the formulation of the optimal control problem. *So operational improvement by actuation should be explored in an optimal control setting.*

5. AN EXAMPLE: DISTILLATION

Here we will use the insight obtained in section 2 to extend the actuation of a distributed process system (distillation column) and the operational improvement will be investigated in an optimal control setting.

In a two-cut splitter a mixture of the components A and B is separated and B is stored in a product tank. In the normal case the distillation column is actuated by the feed F, the boilup V and the reflux L_{10} (see figure 9, left). Clearly the involved phenomenon is mass transfer between liquid and vapor phase. The transfer between the two phases depend on the transfer coefficient, the interface area and the distance from the vapor liquid equilibrium (driving force). The driving force is easy to manipulate by the liquid flow in the downcomers; for example L_9 (see figure 9, right). So the actuation can be extended by adding L_2 - L_9 as DOF. The significant increase in the number of DOF, from three to 11, is a result of extending the distillation column with spatial actuation.

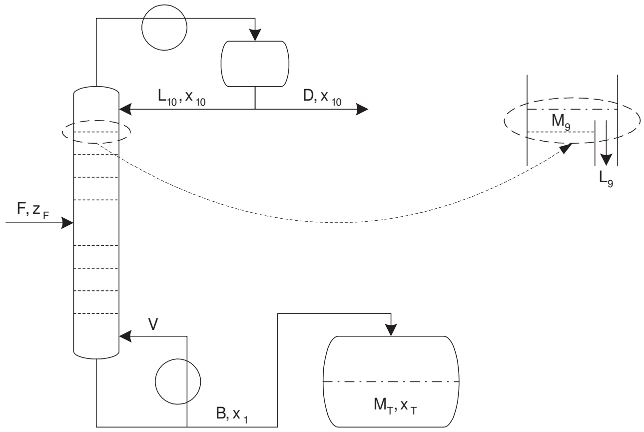

Fig. 9. A distillation system with normal (left) and extended actuation (right).

Both systems were used to solve an optimal control problem. The objective was to minimize $\int_0^2 wF(t)+V(t)dt$ subject to system behavior, operational constraints and the terminal constraints $M_T(2) = 1.1$ and $x_T(2) = 0.2$. The objective reflects the operational cost; feed plus energy, with w being the cost of feed over the cost of energy. Great care was taken to ensure a fair comparison between the normal and extended case. The optimal control problem was solved using dynamic optimization; the simultaneous approach based on an implicit Euler transcription. The implementation was done in the algebraic language GAMS with the solver CONOPT. The normal case is described in detail by Huesman et al. (2007). The results are shown in figure 10. In the case of normal actuation the objective value was 7.2327 while in the case of extended actuation it could at least go as low as 4.6417; this means a considerable improvement of 35%.

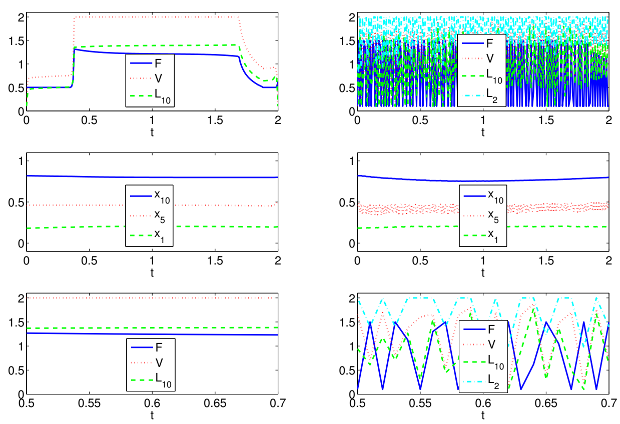

Fig. 10. The distillation system results for normal (left) and extended actuation (right).

Intensified actuation results in, roughly, periodic operation. It has been known since the 1960s that this form of operation (also known as controlled cycling) is attractive, Douglas (1972) gives a nice overview overview of the relevant literature. The superiority of periodic operation was proven analytically and experimentally [4]. The reason for the operational improvement is that a higher time average driving force for mass transfer is obtained with controlled cycling. Further research on periodic operation of distillation columns has resulted in a patent by Lund and Millar (1976) for an innovative downcomer but also in horizontal distillation columns, see Baron and Wajc (1979) and Baron and Barre (1987) for more information.

It is quite instructive to modify the optimal control problem and analyze the results. Three cases will be mentioned briefly below:

(1) If the objective just considers energy cost (minimize $\int_0^2 V(t)dt$) then the operational improvement goes up to 50%. So periodic operation is twice as energy efficient as normal operation.
(2) The operational improvements are largely maintained if only the internal liquid and vapor flows are periodic. So the feed and product flows (distillate and bottom) can be kept constant.
(3) The extended actuation has a significant impact on the economics but very little impact on input/output controllability. In the extended and normal case disturbances are rejected with the same speed.

6. CONCLUSIONS AND FUTURE WORK

Actuation implies the manipulation of fluxes and/or geometry. This insight identifies the domain knowledge that is needed to systematically design actuation for process systems. Fluxes and geometry are both already part of the domain knowledge of chemical engineering but not so much of CPD that focuses more on unit operations. Future research could provide various actuation alternatives for known unit operations. So each unit operation is then analyzed on the deeper detail level of fluxes and geometry for actuation alternatives. This could be combined with looking at the same detail level for process design alternatives, this means a merger of actuation design and process intensification.

The relation between actuation and operational improvement is best explored in an optimal control setting. Compared to a fixed operation mode the operational design space is much larger and also the search through this space is performed by constantly improving optimization techniques. Furthermore any operational limitations can be addressed as constraints in the formulation (up to the point that even certain operation modes can be suppressed). However in the optimal control formulation the important aspect of uncertainty is missing. It is clear that this aspect has to be addressed in some sense in future research.

[4] The experiments also showed that periodic operation allows distillation columns to be operated at 200-300% of normal maximum throughput.

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