INTEGRATING MPC AND RTO IN THE PROCESS INDUSTRY BY ECONOMIC DYNAMIC LEXICOGRAPHIC OPTIMIZATION; AN OPEN-LOOP EXPLORATION

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Introduction

The need for dynamic operation in the process industry is described by Backx et al. [1]. The economics are increasingly driven by the market and this requires flexible supply chains. In such an environment it is much harder to optimize economic performance while maintaining the required product quality and honoring operational constraints. Therefore it is expected that the current industrial state-of-the-art approach for process operation (see figure 1) will prove to be insufficient.

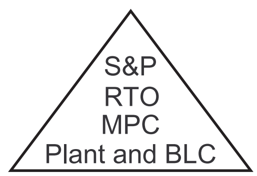

Figure 1 State-of-the-art approach.

The state-of-the-art approach consists of various layers. The lowest layer is the plant with the Base Layer Control (BLC). The latter typically consists of PID controllers and extensions like ratio, override and split range control. The next layer is Model Predictive Control (MPC), a form of model based control that can handle interaction and constraints. The third level is Real Time Optimization (RTO) that optimizes economic performance using steady state models. The final level is Scheduling and Planning (S&P). Planning typically generates economic forecasts and production goals while scheduling basically determines how to execute the chosen plan, the key issue being feasibility. More information on the state-of-the-art approach can be found in Luyben [7] or Marlin [8]. There are a few problems with the state-of-the-art approach which are all related to the fact that RTO uses steady state models. The first thing is that the approach is not general; RTO only supports continuous operation. The second problem is that RTO is slow; model updates can only occur at steady state and this can take a long time, see White [12]. And finally RTO is limited to only steady state improvements; transitions can not be optimized.

Therefore it has been argued by for example Backx et al. [1], Kadam et al. [6] and Rolandi and Romagnoli [10] that MPC and RTO should be integrated "to get the best of both worlds"; Economic Dynamic Optimization (EDO) or as it sometimes called Dynamic Real Time Optimization (DRTO). A considerable amount of work has been done in the area of dynamic process optimization; see for example Biegler [2], Diehl et al. [4] and Schlegel and Marquardt [11]. However this work concentrates on how to solve this type of optimization problems. What remains unanswered is the question what operation results from such an optimization.

This paper will address the last question in an open-loop setting. First we will formulate EDO in a general sense. Then this formulation is used to perform EDO on three process systems (experiments). It will be shown that for each experiment EDO leads to non-unique (multiple) solutions which are handled well by lexicographic optimization. The paper ends with conclusions and directions for future work.

Formulation

The open-loop formulation of EDO takes the shape of an optimization problem. So we must define an objective and a set of constraints. The starting point for the objective is profitability. Standard profitability measures like payback period, net present value or internal rate of return, see Brennan [3], cover the whole project period (initiation, design, construction, operation and dismantling) which means a few to 20 years. Because of these long periods the time value of money must be taken into account. However it will become clear in the next paragraph that the time horizon of EDO is less than four weeks. So there is no need to compensate for the time value of money and a straightforward profit *P* can be maximized:

$$P = \underbrace{\text{revenues}}_{\text{prices}\cdot\text{quantity products}} - \underbrace{\text{total costs}}_{\text{fixed}+\text{variable}} - \text{taxes}^{1} \qquad (1)$$

By definition fixed and variable costs are respectively independent and dependent on product quantity. It should be noted that the fixed costs and taxes are not under the influence of operation. So in an optimization problem these terms are constants and maximization of equation (1) simplifies to the maximization of operational profit:

$$OP = \text{prices} \cdot \text{quantity products - variable costs} \qquad (2)$$

With respect to the constraints two types are obvious; plant behavior and operational constraints. However, also so-called "scheduling constraints" are needed. In the simplest case this type boils down to the required product quantity and quality at a time t_f in the future. In the more elaborate case it can be a number of required quantities and qualities at times t_{f1}, $t_{f2}\ldots t_{fn}$. The last point in the future t_{fn}, equals the scheduling horizon which is normally between one to four weeks. For this reason the time horizon of EDO is less than four weeks. The scheduling constraints provide the necessary link with scheduling and therefore possible interaction with other plants on the site (shared utilities, tanks etc.). To summarize; economic dynamic process optimization can be formulated as the following optimization problem:

$$\max \int_0^{t_f} (OP)\,dt \quad \text{s.t.} \begin{cases} \text{plant behavior} \\ \text{operational limitations} \\ \text{scheduling constraints} \end{cases} \qquad (3)$$

If the required product quantity is not allowed to vary (so the corresponding constraint is an equality rather than an inequality) then problem (3) can be reduced to:

[1] According the viewpoint of the plant manager taxes have to be subtracted.

$$\min \int_0^{t_f} (OC)\,dt \quad \text{s.t.} \begin{cases} \text{plant behavior} \\ \text{operational limitations} \\ \text{scheduling constraints} \end{cases} \tag{4}$$

Here OC stands for operational costs. Problems (3) and (4) can also be expressed mathematically:

$$\min_u \int_0^{t_f} F_1\,dt \quad \text{s.t.} \begin{cases} dx/dt = f(x,y,u,t),\; x(0) = x_0 \\ h(x,y,u,t) = 0 \\ g(x,y,u,t) \geq 0 \end{cases} \tag{5}$$

Here F_1 stands for -*OP* (note the minus sign) or *OC*, *x* for state variables, *y* for algebraic variables and *u* for inputs or Degrees Of Freedom (DOF). All variables are functions of time. Typically all relationships in problem (5) are linear except for those that are related to plant behavior. So this problem constitutes a Non-Linear Program (NLP).

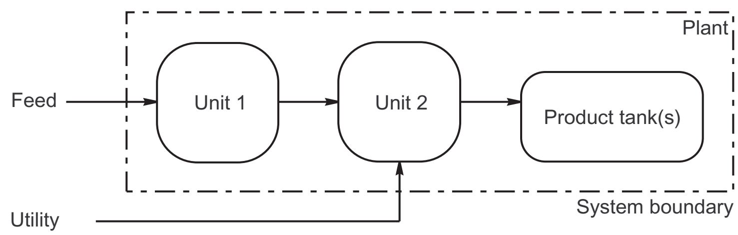

Figure 2 A plantwide system boundary.

The economic objective has consequences for the system boundary. Normally prices of flows between feed and product, so-called intermediate prices, are unknown. See for example figure 2, the price of the flow between unit 1 and 2 is normally not known. The system boundary should be chosen such that intermediate prices are not needed. This means that a plantwide system boundary is adopted. It should be noted that the boundary also includes product tank(s). This allows for dynamic improvement; the product flow to the tank may vary freely between operational limits and the same might even apply to the product quality.

Experiments

Single Tank

The first system is just a product tank (see figure 3).

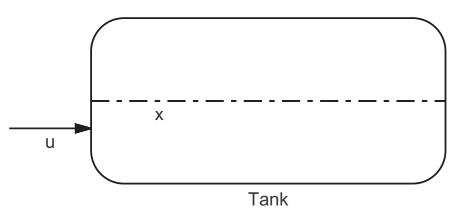

Figure 3 A product tank.

The tank should be filled at minimum cost to at least a certain minimum level given some input constraints:

$$\min_u \int_0^2 u(t)dt \quad \text{s.t.} \begin{cases} dx/dt = u(t),\ x(0) = 0 \\ 0 \leq u(t) \leq 10 \\ x(2) \geq 5 \end{cases} \tag{6}$$

Problem (6) was solved by means of the simultaneous approach. The transcription is based on implicit Euler. The implementation was done in the algebraic language GAMS, the used solver was CONOPT. The result is shown in figure 4a.

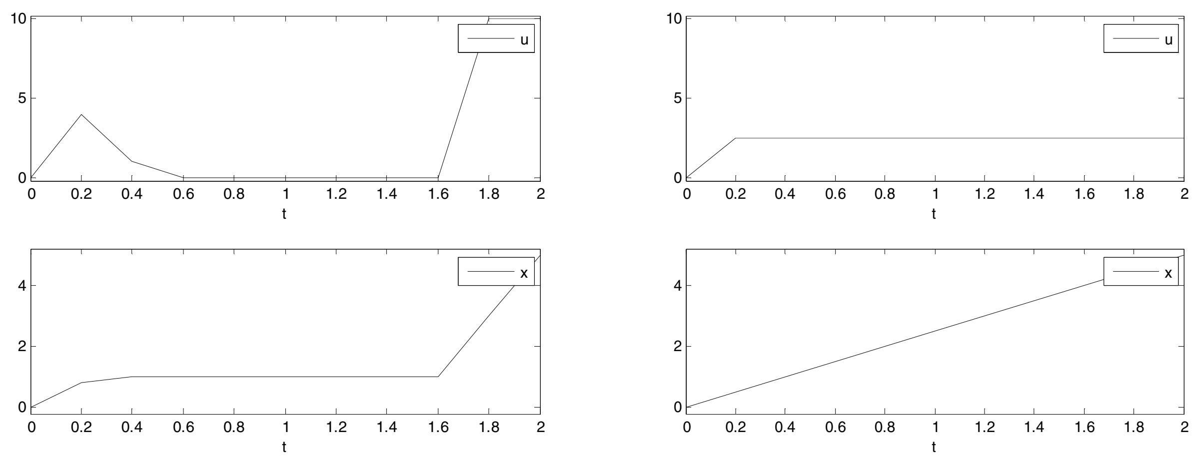

Figure 4a (left) and b (right) The result of the 1st and 2nd stage single tank problem.

Looking at the result the question rises if this is the only possible solution. A simple way to check this is by changing the initial guess for the input and/or state trajectories. The effect is that these trajectories change but that the objective value stays the same. This implies that the optimal trajectories are not unique; there exist multiple solutions.

Stirred Tank Reactor and Tank

This system includes a Stirred Tank Reactor (STR)[2] besides a tank (see figure 5).

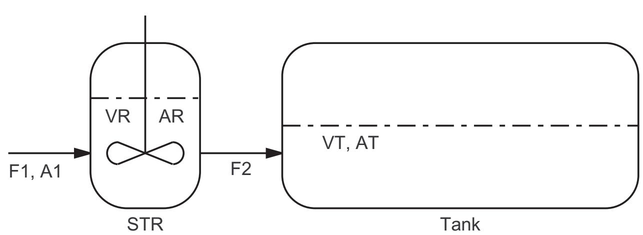

Figure 5 A STR and a product tank.

[2] A STR is a continuous stirred tank reactor of which the level is allowed to vary.

The discussion of this experiment will be quite brief since it was already described in detail in Huesman et al. [5]. In the STR the reaction A to B takes place. The product B is stored in the tank. The following assumptions are made:

- The reaction is first order in A.
- The density is constant.
- The STR and tank are both well-mixed.

This system is described by four nonlinear differential equations with four state variables (VR, VT, AR and AT) and two DOF (F1 and F2). The objective is to minimize the integrated value of (vF1 + VR) over 2 time units while producing a certain amount of product; VT(2) = 2.1 of a certain quality; AT(2) = 0.05. The objective reflects the operational costs; feed plus stirring (the stirring power is assumed to be proportional to the reactor volume). The parameter v represents the ratio cost of feed over cost of stirring. The optimization was solved in the same way at the single tank experiment. The result is shown in figure 6a.

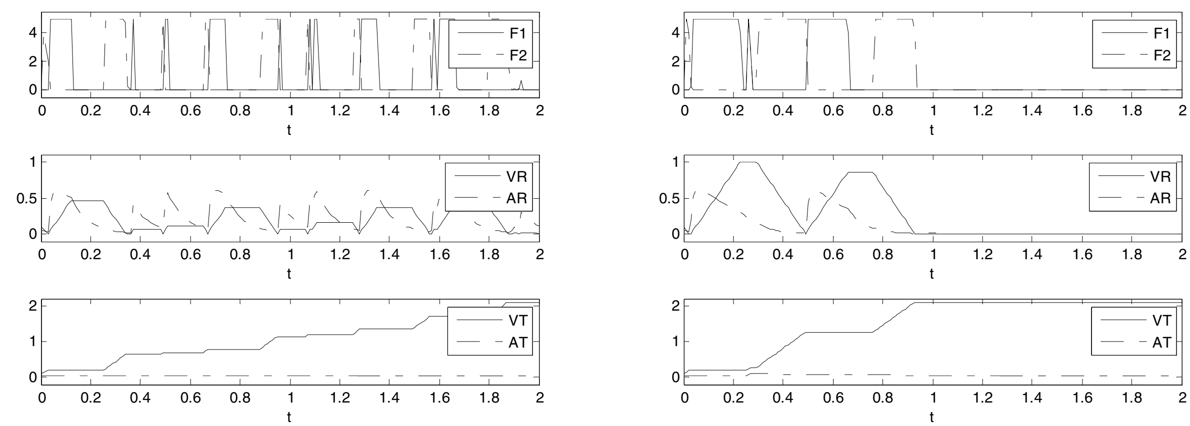

Figure 6a (left) and b (right) The result of the 1st and 2nd stage STR and tank problem.

The STR is filled and emptied several times; so EDO prefers batch operation. From a reactor engineering point of view this result was to be expected, batch operation leads to a high average reactant concentration which results in a low average reactor volume and therefore low cost. The timing of the batches looks arbitrary. And also in this case changing the initial guess for the input and/or state trajectories reveals the existence of multiple solutions.

Distillation Column and Tank

In the last system the STR is replaced by a Distillation Column (DC) with eight trays, see figure 7.

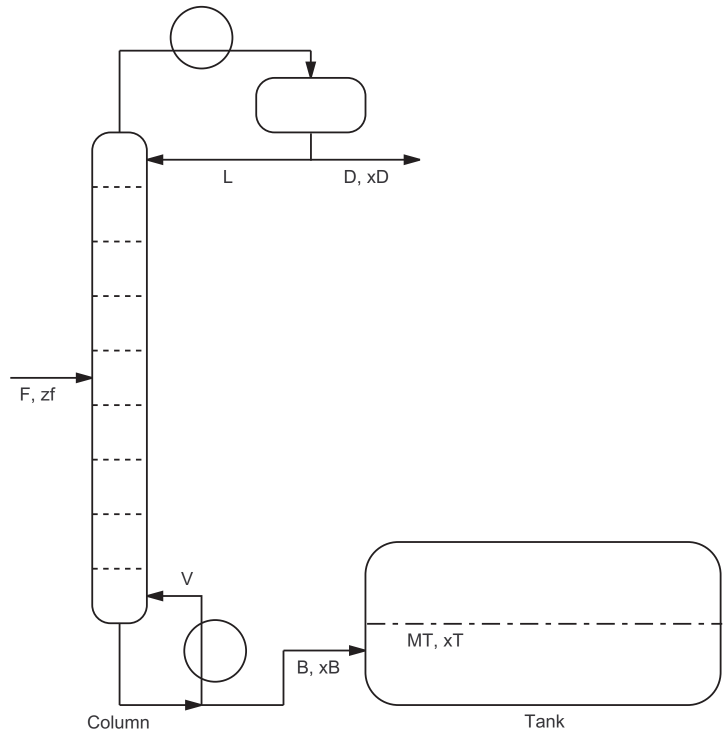

Figure 7 A DC and a product tank.

Also this experiment is described in detail in Huesman et al. [5]. The heavy component (product) is stored in a tank while the light component leaves the system. The following assumptions are made:

- The vapor phase can be neglected.
- Trays, top and bottom inventory are well-mixed.
- Outgoing flows on a tray are in equilibrium which is described by constant relative volatility.
- The liquid molar hold-up on each tray and in top and the bottom inventory is constant.
- The liquid and vapor molar flows are constant (constant molar overflow).
- The tank is well-mixed.

Trays, top and bottom inventory are all considered compartments. So in total there are ten compartments. The compartments are numbered from the bottom to the top, so $xB = x1$ and $xD = x10$. This system is described by 12 nonlinear differential equations with 12 state variables (x1 to x10, xT and MT) and three DOF (F, V and L). The objective is to minimize the integrated value of (wF + V) over 2 time units while producing a certain amount of product; $MT(2) = 1.1$ of a certain quality; $xT(2) = 0.2$. Again the objective reflects the operational costs; feed plus utility, the parameter w represents the ratio cost of feed over cost of steam. This dynamic optimization was solved in the same way as the single tank experiment. The result is shown in figure 8a.

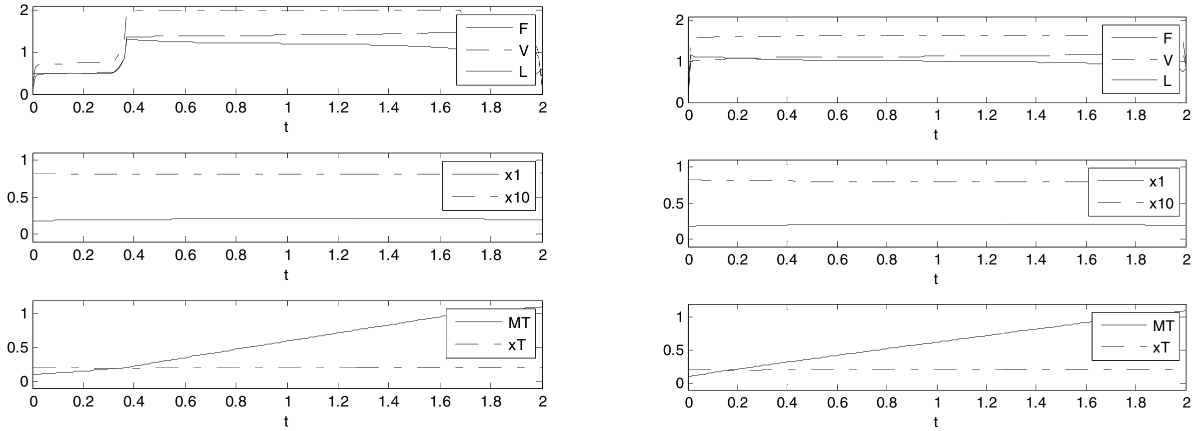

Figure 8a (left) and b (right) The result of the 1st and 2nd stage DC and tank problem.

It is clear that F rises rapidly. Closer inspection reveals that this also happens to V and L. As a matter a fact the ratios V over F and L over F remain constant over time. So EDO prefers constant ratios and from a distillation point of view this is not a complete surprise. Repeating the exercise of changing the initial guess for the input and/or state trajectories again reveals the existence of multiple solutions.

Lexicographic Optimization

Figure 9 shows the graph of a function with a unique and multiple solutions. For one decision variable the existence of multiple solutions seems artificial however Huesman et al. [5] show that for two and more decision variables cases are easy to construct.

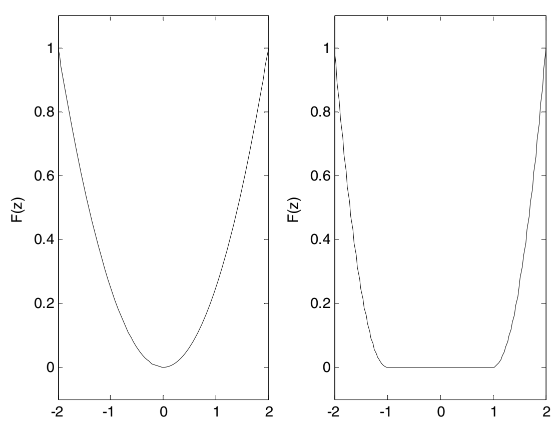

Figure 9 A unique solution (left) and multiple solutions (right).

Multiple solutions can be analyzed by means of a SVD (Singular Value Decomposition) of the Jacobian of the active first order KKT (Karush Kuhn Tucker) conditions around the optimal point. Let J be this Jacobian and Δz be small changes in the decision variables, then multiple solutions exist if:

$$J\Delta z = USV^T \Delta z = 0 \quad (7)$$

In other words one or more singular values should be zero. Figure 10 shows the result for the single tank example. Note that indeed a number of singular values are zero. By the way this analysis provides more information; for example the dimension of the multiple solutions space.

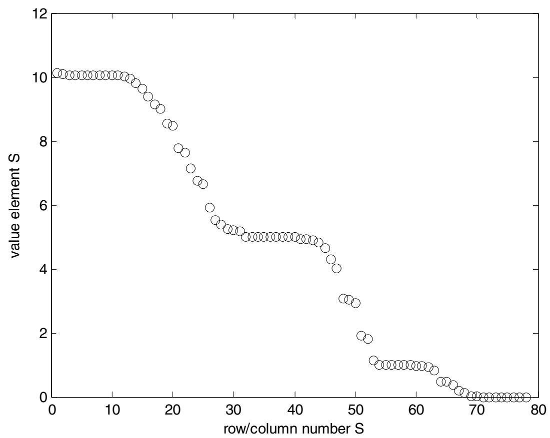

Figure 10 The singular values of the Jacobian J for the single tank problem.

There are two reasons why the final solution should be locally unique:

1. In a closed-loop setting EDO will be performed repeatedly. This can easily lead to "jumping around the multiple solutions space".
2. The existence of multiple solutions implies that there are still DOF left. So there is an opportunity to perform another optimization. Of course this optimization should be based on a different objective and it should not sacrifice economic performance (too much).

The last reason strongly suggests the use of lexicographic optimization; a form of multiobjective optimization, see Miettinen [9]. For two objectives F_1 and F_2 it boils down to:

$$\min F_1(z) \;\; \text{s.t.} \begin{cases} h(z) = 0 \\ g(z) \le 0 \end{cases} \Rightarrow \text{a solution } z^* \qquad \min F_2(z) \;\; \text{s.t.} \begin{cases} h(z) = 0 \\ g(z) \le 0 \\ F_1(z) \le (1+S)\cdot F_1(z^*) \end{cases} \quad (8)$$

So the overall optimization is done in two stages. The 1st stage involves an economic objective F_1 and determines the best economic performance F_1*. The 2nd stage is based on a different objective F_2 and only uses the remaining DOF because of the extra constraint on economic performance. The last constraint can be relaxed with the parameter *S*.

Is lexicographic optimization not somewhat complex and computationally expensive? In order to answer that question lets consider the alternative that is used in MPC; regularization. In MPC regularization is provided by the term $\Delta u^T R \Delta u$, with Δu being the input moves and *R* a weighing matrix. For regularization to work properly the matrix *R* must be tuned carefully in order to balance regularization with the original objective. In the case of lexicographic optimization only one scalar parameter *S* needs to be specified and this is straightforward since its influence is completely transparent. By the way the computational effort of the 2nd stage will be small provided that this stage continues where the 1st stage stopped (hot-start of the 2nd stage). To summarize; compared to regularization lexicographic optimization is less complex and about comparable in computational effort.

Lexicographic optimization was applied to the three experiments previously discussed. For the choice of the 2nd objective and the parameter *S* see table 1.

Table 1 Details of the 2nd stage optimization of the three experiments.

Experiment	**2nd objective**	***S***
Single tank	Achieve steady operation: $\min \int_0^2 \left((u(t)-5)^2 \right) dt$	0
STR and tank	Realize schedule in minimal time: $\min \int_0^2 \left((VT(t)-4)^2 + (AR(t)-0)^2 \right) dt$	0.03
DC and tank	Achieve steady operation: $\min \int_0^2 \left((F(t)-3)^2 + (V(t)-3)^2 + (L(t)-3)^2 \right) dt$	0.001

The hot start of the 2nd stage was implemented in GAMS by using two model and two solve statements. The results are shown in figure 4b, 6b and 8b. In all cases lexicographic optimization resulted in considerable changes of the optimal trajectories and unique solutions. Note that the remaining DOF were really utilized by the lexicographic approach. For example in the STR and tank experiment the time needed to realize the schedule was halved.

Conclusions and Further Work

A general well-motivated formulation of EDO has been given. It was shown that this formulation does not intrinsically fix all DOF. It was also shown that remaining DOF can be utilized by lexicographic optimization.

Future work will focus on the background of multiple solutions (why and when do they appear?), a general approach for the 2nd objective (what are sensible objectives and how to formulate them?) and extension of the open-loop to the closed-loop case.

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