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DEGREES OF FREEDOM ANALYSIS OF ECONOMIC DYNAMIC OPTIMAL PLANTWIDE OPERATION

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Improving the operation is an attractive option for the process industry to deal with increased competition. In this paper a general dynamic optimization framework is proposed that aims to improve plantwide operation in an economic sense. The term general means that it is based on dynamic operation in which any operational constraints can be accommodated. One would expect economic optimization to utilize all available degrees of freedom. However it is shown that this is normally not the case, so this leaves the possibility open to do further optimization.

Keywords: Degrees-of-freedom, Dynamic, Economic, Plantwide, Optimization.

1. INTRODUCTION

Due to globalisation the process industry is faced with increased competition. This has resulted in pressure on the margins and the process industry has to find ways to secure and/or improve its economic performance. This can be done by changing the design, the operation or a combination of both. Certainly for existing plants improving the operation is an attractive "low-cost" option.

Operational improvement requires the availability of all possible process Degrees Of Freedom (DOF). These can be calculated by:

$$\#DOF = \#NV - \#NE \qquad (1)$$

In (1) *#NV* stands for the number of variables and *#NE* for the number of equations. Equation (1) easily leads to errors; a small number is determined by the subtraction of two large numbers. Therefore easier methods have been developed by Pham (1994), Ponton (1994) and Luyben (1996). The last method boils down to the fact that the number of DOF equals the number of flows that can be manipulated. This method will be used in this paper. The various methods are compared by Murthy Konda, Rangaiah and Krishnaswamy (2006).

While improving operation one needs to have a clear overview of all operational objectives. A good starting point is provided by plantwide control. Plantwide control was initiated by Buckley (1964), who stated that the main objective of a plant is to produce the required quantity and quality. Furthermore Buckley introduced the concept of material balance control and discussed its interaction with quality control. The interest in the subject increased during the 90's and this resulted in a text book by Luyben, Tyreus and Luyben (1998). In their book they discuss the influence of recycles and present a plantwide control design procedure. A review on the subject of plantwide control is provided by Larsson and Skogestad (2000). There is mutual agreement that the plantwide control objectives can be summarized as:

1) Stay within operational constraints.
2) Realize the required quantity and quality.
3) Optimize economic performance.

It should be mentioned that plantwide control only considers continuous operation. Also the attention for the third plantwide objective (optimize economic performance) has been very limited. So the focus of plantwide control has been on feasibility. Plantwide control deals with DOF in a straightforward way; for each DOF there is normally one control objective. In this way all DOF are fixed.

According to White (1999) economic process optimization dates back almost 50 years. The current state of the art is Real Time Optimization (RTO). Since RTO is in fact steady state optimization it is not compatible with batch operation. It has been recognized that RTO is slow since each optimization has to be proceeded by a steady state. The last two decades there has been a substantial amount of work on dynamic optimization, see Biegler (2004). However the main focus has been on how to perform dynamic optimization. The same goes for batch optimization; see Méndez, *et al.* (2006). It should be noted that “the state of the art” for batch operation are recipes that are not optimal since their development is normally done under time pressure.

To summarize the discussion above:

- The process industry needs to improve its economic performance.
- Plantwide control only considers continuous operation and pays little attention to economic performance.
- RTO can only be used to improve the economic performance of continuous operation. Another limitation is that RTO is slow.
- The economic performance of continuous as well as batch operation can be *improved dynamically*. This improvement can be explored and exploited by dynamic optimization.
- Most of the work done on dynamic optimization focuses on how to perform dynamic optimization rather than the possible economic benefits.

To bridge the gap between economic performance and dynamic optimization this paper focuses on the following question:

How to frame dynamic optimization such that we can expect improved operation in an economic sense?

In this paper such a general framework will be proposed. The term general means that it is based on dynamic operation in which any operational constraints can be accommodated. The framework deals with the DOF in an optimization rather than a control context. Therefore special attention will be paid to the question:

Does dynamic optimization with an economic objective utilize all DOF?

If not all DOF are utilized then there is the possibility to do further optimization. This paper will only consider optimization in an off-line setting.

In the rest of this paper first the framework is presented. Then the framework is investigated in two numerical experiments. The last section summarizes the conclusions and suggests directions for future work.

2. DYNAMIC OPTIMIZATION FRAMEWORK

The framework adopts a plantwide system boundary. In this way we avoid the need to know intermediate prices; the flows associated with intermediate prices simply fall within the system boundary.

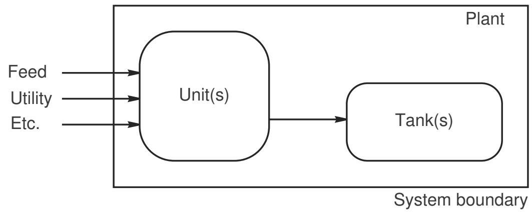

Figure 1. A visualization of the proposed framework.

The framework incorporates product tank(s), see figure 1. This allows for dynamic improvement in the sense that at least the product flow to the tank does not have to be constant. If the product quality to the tank is allowed to vary depends on the ease of mixing. For low viscosity products “on spec” mixing in the tank is certainly an option, but high viscosity products should be produced directly “on spec”. Note that the inclusion of products tank(s) also implies that the framework supports continuous as well batch operation. In the case of batch the unit(s) and the tank(s) are just completely integrated.

The plantwide control objectives can be reformulated as a dynamic optimization problem:

$$\text{min cost} \qquad s.t.\begin{cases}\text{plant behaviour}\\ \text{required quantity and quality}\\ \text{operational constraints}\end{cases} \tag{2}$$

Or mathematically:

$$\min_{u} \int_{o}^{t_f} F(x,y,u)dt \qquad s.t.\begin{cases} dx/dt = f(x,y,u,t),\ x(0)=x_0\\ h(x,y,u,t)=0\\ g(x,y,u,t)\geq 0\end{cases} \tag{3}$$

In problem (3) x stands for state variables, y for algebraic variables and u for inputs. Normally all these variables are functions of time. The variable t_f denotes the finite horizon. The horizon as well as the required quantity and quality are supplied by scheduling. This facilitates integration with scheduling but it also means that the product is handled as a constraint rather then as a part of the economic objective (in the form of revenues). So the economic objective is a cost function; it typically takes into account the cost of the flows that cross the system boundary (feed, utilities, etc.).

As explained in the introduction the number of operational DOF equals the number of flows that can be manipulated. So within the proposed framework the number of DOF equals the number of flows that cross the system boundary plus the number of flows that can be manipulated within the system boundary. In other words the objective contains fewer variables than DOF; the objective is sparse.

Often the objective is linear, the same goes for the required quantity and quality and the operational constraints. However the plant behaviour is normally non-linear and for that reason problem (2) and (3) are non-linear optimization problems.

3. EXPERIMENT 1, STIRRED TANK REACTOR AND TANK

This system consists of a Stirred Tank Reactor (STR) and a tank (see figure 2). In the STR the reaction A to B takes place. The product B is stored in the tank. The following assumptions are made:

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

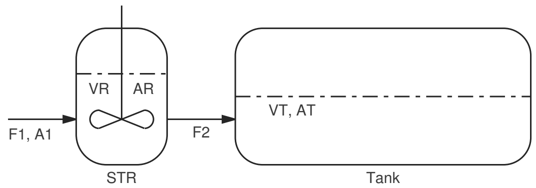

Figure 2. A STR and a tank.

From a total mass balance over the STR and the tank we can derive:

$$\frac{dVR}{dt} = F1 - F2 \qquad \frac{dVT}{dt} = F2 \tag{4}$$

Repeating the exercise for a molar balance for component A gives:

$$\frac{dAR}{dt} = \frac{F1}{VR}(A1 - AR) - kAR \qquad \frac{dAT}{dt} = \frac{F2}{VT}(AR - AT) \tag{5}$$

So the total system is described by four differential nonlinear equations. Furthermore we have four state variables (*VR*, *VT*, *AR* and *AT*) and two DOF (*F1* and *F2*). The objective is to minimise the integrated value of *(vF1 + VR)* over 1 hour while producing a certain amount of product (VT_{final} = 2.1) of a certain quality (AT_{final} = 0.05). The objective reflects the total operating costs; feed plus stirring (the stirring power is assumed to be proportional to the reactor volume). The parameter *v* represents the ratio $\text{cost}_{\text{feed}}$ over $\text{cost}_{\text{stirring}}$. For values of parameters, initial conditions etc. see table 1 in the appendix.

The dynamic optimization was solved using the simultaneous approach, see Biegler (1984). The differential equations (4) and (5) were discretized by an implicit Euler scheme in which the time step *Dt* was fixed at 0.01 hours. For example using *N* grid points to discretize the total mass balance over the STR gives:

$$Dt = \frac{t_f - 0}{N-1}, \text{ for } i \in \{2,3,4...N\}: \qquad \frac{VR(i) - VR(i-1)}{Dt} = F1(i) - F2(i) \tag{6}$$

The implementation was done in an algebraic language (GAMS), the solver used was CONOPT. The result is shown in figure 3. The calculation time for this problem was around 1 second (Windows XP professional, 3.2 GHz and 1 Gb RAM).

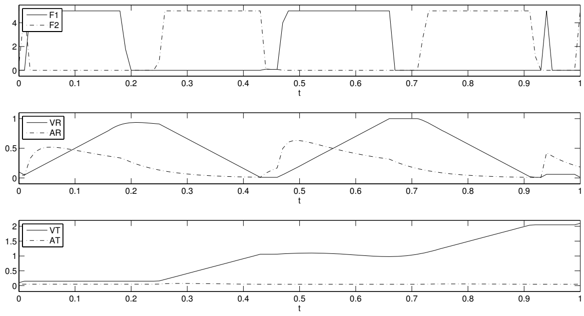

Figure 3. The optimal trajectories for the STR and tank example. The horizon is 1 hour.

The solution is almost periodic. The STR is filled and emptied twice; so two batches are performed. From a reactor engineering point of view this result was to be expected by choosing batch operation the average reactant concentration is high which results in a low reactor volume. Note that the framework is actually capable of “selecting” batch operation.

Now let’s increase the horizon to 2 hours while keeping the rest the same. Figure 4 shows the result.

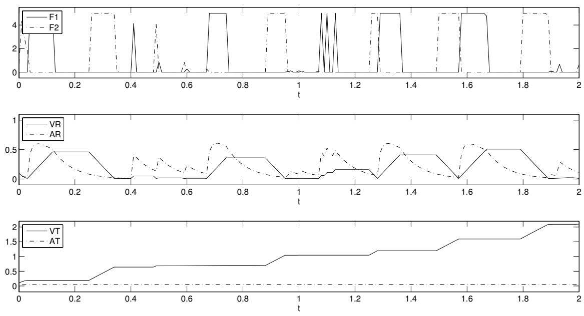

Figure 4. The optimal trajectories for the STR and tank example. The horizon is 2 hours, the initial guess for all decision variables is set to 0.5.

Although the STR is still operated in a batch way, the solution is no longer periodic. As a matter a fact changing the initial guess for the decision variables changes the trajectories without affecting the objective value (see figure 5).

So the optimal trajectories are to a certain extent arbitrary. This result can be explained by the existence of “multiple solutions”, see figure 6. This figure implies that there is an optimal constrained subspace perpendicular to the objective gradient:

$$(x2^* - x1^*) \cdot \nabla F = |\Delta x^*| . |\nabla F| . \cos\theta = 0 \tag{7}$$

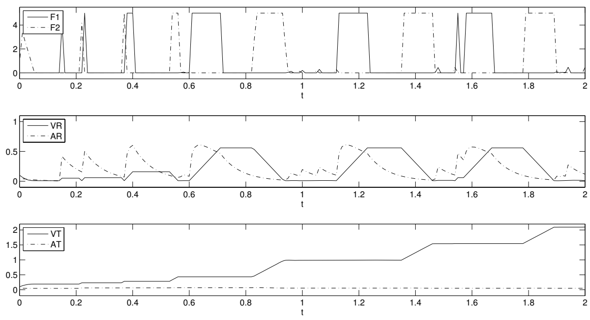

Figure 5. The optimal trajectories for the STR and tank example. The horizon is 2 hours, the initial guess for all decision variables is set to 1.0.

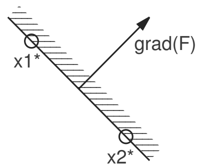

Figure 6. The existence of multiple solutions, x1* and x2* are optimal solutions in the decision space.

Using the data that correspond to figure 4 and 5 gives an inproduct of -0.0113 and an angle of 90.003°. Especially the angle confirms the explanation. Multiple solutions result from the fact that we have a sparse linear objective and linear inequality constraints. This can be illustrated by a simple problem:

$$\max_{x1,\,x2,\,x3} x2 \qquad s.t.\begin{cases} x1x3 = 0.5 \\ 0 \le x1 \le 1 \\ 0 \le x2 \le 1 \\ 0 \le x3 \le 1 \end{cases} \tag{8}$$

This optimization problem has 3 decision variables, 1 non-linear equality, 2 DOF, a sparse linear objective and 3 linear inequalities. Figure 7 shows the set of multiple solutions; the black curve in the shaded plane.

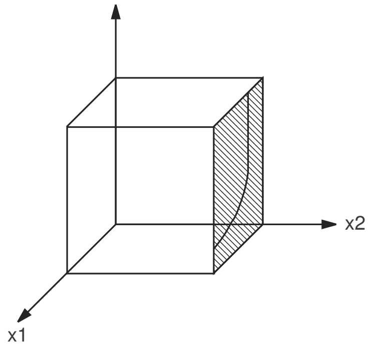

Figure 7. The solution of optimization problem (8).

Basically this means that *a realistic economic objective does not utilize all DOF*.

4. EXPERIMENT 2, DISTILLATION COLUMN AND TANK

The STR is now replaced by a binary Distillation Column (DC) with eight trays (see figure 8).

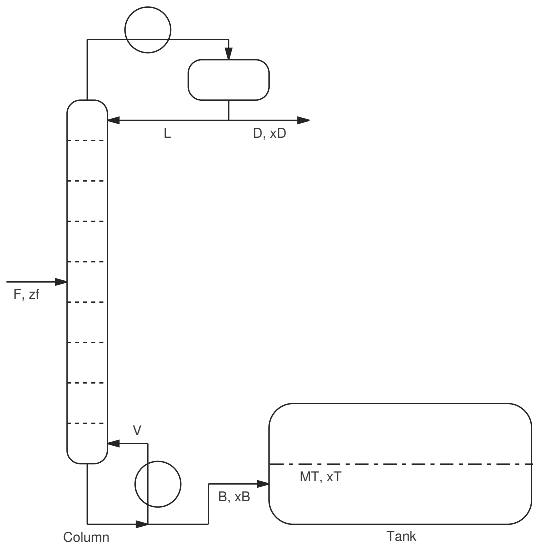

Figure 8. A DC and a tank.

The heavy component (product) is stored in a tank; the light component leaves the system. The modelling closely follows Skogestad, 1997. The following assumptions are made:

1) The vapour phase can be neglected.
2) Trays are well-mixed. We assume the top and the bottom inventory to be well-mixed as well.
3) Outgoing flows on a tray are in equilibrium.
4) The liquid molar hold-up on each tray is constant. The same goes for the top and the bottom inventory.
5) The liquid and vapour molar flows are constant (constant molar overflow).
6) The tank is well-mixed.

Trays, top and bottom inventory are all considered compartments. So in total there are 10 compartments. The compartments are numbered from the bottom to the top. The numbering of the mole fractions is explained in figure 9.

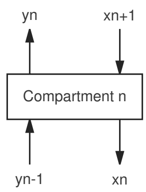

Figure 9. Numbering of the mole fractions.

The equilibrium on a tray is given by:

$$yn = \frac{\alpha\, xn}{1 + (\alpha - 1)xn} \tag{9}$$

By the way the numbering implies that $xB = x1$ and $xD = x10$. From a molar balance (total and light component) over all compartments we obtain:

$$\frac{dx10}{dt} = \frac{Vy9 - Lx10 - Dx10}{M10}$$

for $i \in \{6,7,8,9\}$:

$$\frac{dxi}{dt} = \frac{Vy(i-1) + Lx(i+1) - Vyi - Lxi}{Mi}$$

$$\frac{dx5}{dt} = \frac{Fzf + Vy4 + Lx6 - Vy5 - (L+F)x5}{M5} \quad (10)$$

for $j \in \{2,3,4\}$:

$$\frac{dxj}{dt} = \frac{Vy(j-1) + L'x(j+1) - Vyj - L'xj}{Mj}$$

$$\frac{dx1}{dt} = \frac{L'x2 - Vy1 - Bx1}{M1}$$

$$L' = L + F, \quad B = L + F - V, \quad D = V - L$$

A molar balance (total and light component) over the tank gives:

$$\frac{dMT}{dt} = B$$
$$\frac{dxT}{dt} = \frac{B(xB - xT)}{MT} \quad (11)$$

So the system has 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 hours while producing a certain amount of product (VT_{final} = 1.1) of a certain quality (AT_{final} = 0.2). Again the objective reflects the total operating costs; feed plus utility, the parameter *w* represents the ratio $cost_{feed}$ over $cost_{steam}$. For values of parameters, initial conditions etc. see table 2 in the appendix.

This dynamic optimization was solved in exactly the same way as the STR and tank example. The result is shown in figure 10.

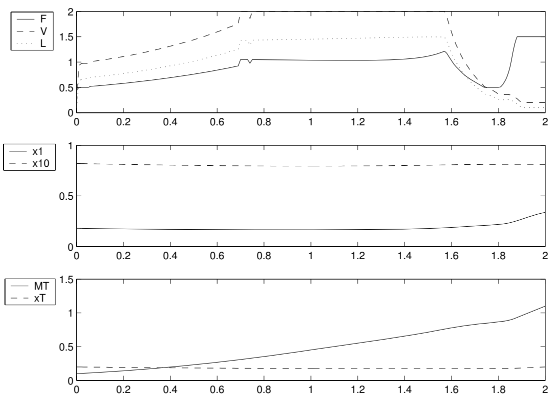

Figure 10. The optimal trajectories for the DC and tank example.

The calculation time for this problem was around 1 minute (Windows XP professional, 3.2 GHz and 1 Gb RAM).

Figure 10 shows that the bottom is left at a high mole fraction; 0.34 (near the end of the horizon the bottom is “flushed out”). Figure 11 shows what happens if we repeat the dynamic optimization with the extra constraint; xB = 0.2 at t = 2.0

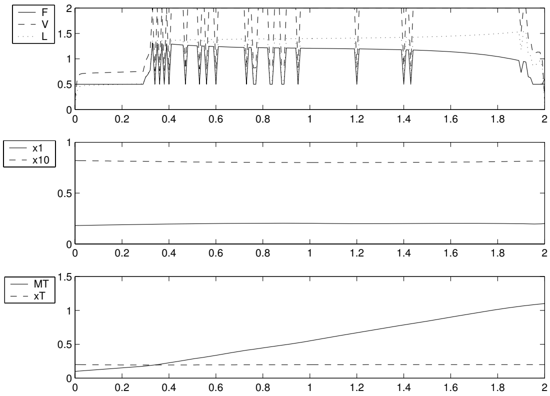

Figure 11. The optimal trajectories for the DC and tank example with the constraint xB = 0.2 at t = 2.0.

Figure 11 shows that *F* drops and rises rapidly several times. Closer inspection reveals that this also happens to *V* and *L*. As a matter a fact during these transients the ratio *V* over *F* and *L* over *F* remains constant. This conclusion is also supported by figure 10. So in this example neither continuous or batch operation but constant ratios are “selected”.

Also in this case changing the initial guess for the decision variables changes the trajectories without affecting the objective value. So again this means that the economic objective did not utilize all DOF.

6. CONCLUSIONS AND FUTURE WORK

A general dynamic optimization framework is proposed. The term general refers to the fact that it can accommodate any operational constraints. The framework is characterized by:

- An economic cost objective.
- A plantwide system boundary that includes product tanks.
- A finite time horizon and constraints with respect to product quantity and quality.

The framework produces valuable results; for the STR and tank experiment it “selected” batch operation while for the DC and tank example it revealed that certain ratios should be kept constant.

It is shown that normally the framework does not utilize all DOF (due to combination of a sparse linear objective and linear inequality constraints), so this leaves the possibility open to do further optimization.

Future work will focus on “further optimization”. One possibility is to extend the economic objective with the variable t_f. This variable can be associated with economic depreciation. Another possibility is to use hierarchical optimization. In the first optimization step the best economic performance is determined by the proposed framework. In the second optimization step a unique solution is selected from the set of multiple solutions. This implies that the second optimization does not affect the economic performance. The objective used in the second step expresses an operational preference for example; minimize deviation from a known reference solution.

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APPENDIX

Table 1 Values of parameters, initial conditions and decision variables for experiment 1.

Parameters		Initial conditions	
A1	1	*VR*	0.1
k	14.9787	*AR*	0.05
v	2	*VT*	0.1
		AT	0.05

Decision variables	Low limit	Initial guess	High limit
F1	0	0.5	5
F2	0	0.5	5
VR	0.01	0.5	1
AR	0	0.5	1
VT	0.01	0.5	5
AT	0	0.5	1

Table 2 Values of parameters, initial conditions and decision variables for experiment 2.

Parameters		Initial conditions	
α	1.68	*x1*	0.1805
zf	0.5	*x2*	0.2522
M1	0.375	*x3*	0.3254
M2...9	0.002	*x4*	0.3942
M10	0.375	*x5*	*0.4539*
w	2	*x6*	*0.5038*
		x7	*0.5673*
		x8	*0.6439*
		x9	*0.7299*
		x10	*0.8195*
		MT	*0.1*
		xT	*0.2*

Decision variables	Low limit	Initial guess	High limit
F	0.5	1	1.5
V	0.1	2	2.0
L	0.1	1.5	2.0
D	0.1	0.5	2.0
B	0.1	0.5	2.0
x1	0.01	0.1805	1
x2	0.01	0.2522	1
x3	0.01	0.3254	1
x4	0.01	0.3942	1
x5	0.01	0.4539	1
x6	0.01	0.5038	1
x7	0.01	0.5673	1
x8	0.01	0.6439	1
x9	0.01	0.7299	1
x10	0.01	0.8195	1
y1	0.01		1
y2	0.01		1
y3	0.01		1
y4	0.01		1
y5	0.01		1
y6	0.01		1
y7	0.01		1
y8	0.01		1
y9	0.01		1
y10	0.01		1
MT	0.01	0.5	3
xT	0	0.5	1