Control structure selection for Reactor, Separator and Recycle Process

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Abstract

We consider control structure selection, with emphasis on "what to control", for a simple plant with a liquid phase reactor, a distillation column and recycle of unreacted reactants. Plants of this kind have been studied extensively in the plantwide control literature. Our starting point is a clear definition of the operational objectives, constraints and degrees of freedom. Active constraints should be controlled to optimize economic performance. This implies for this case study that reactor level should be kept at its maximum, which rules out many of control structures proposed in the literature from being economally attractive. Maximizing the reactor holdup also minimizes the "snowball effect". The main focus is on the selection of a suitable controlled variable for the remanining unconstrained degree of freedom, where we use the concept of self-optimizing control, which is to search for a constant setpoint strategy with an acceptable economic loss. Both for the case with a given feedrate where the energy costs should be minimined, and for the case where the production rate should be maximized, we find that a good controlled variable is the reflux ratio L/F. This applies to single-loop control as well as multivariable model predictive control.

1 Introduction

A common feature of many chemical processes is the presence of recycle. Variations of a plant with reaction, separation and mass recycle, see Figure 1, have been extensively studied in the literature (with different parameters, with and without a distillation column).

Gilliland *et al.* (1964) used this plant to study how the dynamics and steady state behavior are changed by the positive feedback introduced by the recycle. Papadourakis *et al.* (1987) studied the changes in steady-state RGA for the distillation column caused by introducing the recycle. Price and Georgakis (1993) found that control of internal compositions, either distillate or reactor composition, helps the control of bottom composition. Luyben (1993abc,1994) followed up Gilliland's points and focused on the high sensitivity that the recycle flowrate in some cases has to the feed-flowrate. He

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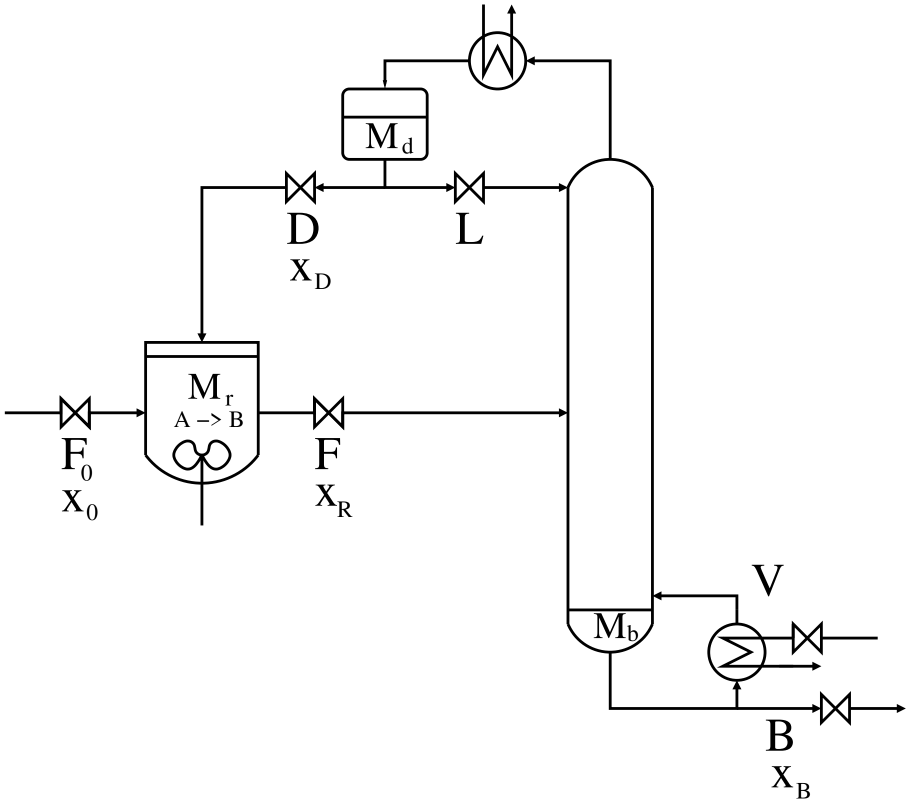

Figure 1: Reactor, separator (distillation) and recycle process.

called this the "snowball effect", and as a remedy proposed to let the reactor holdup vary and as a generic rule proposed that "one flowrate somewhere in the recycle loop should be flow controlled" (Luyben 1993*b*) Wu and Yu (1996) proposed that a better way of avoiding snowballing, and constant reactor composition.

The recycle plant in Figure 1 has four degrees of freedom at steady state: one for the throughput (feedrate F_0), one for the reactor (holdup M_r) and two for the distillation column (e.g. reflux and boilup), see also Table 2. In the literature several alternative sets of controlled variables have been proposed for the case with a given feedrate F_0 and given (and controlled) product composition x_B:

- "Conventional" (denoted x_D in the following): Control of M_r and x_D (fixed reactor holdup and "two-point" distillation column control).
- "Luyben's structure" (LS) with varying reactor holdup: Control of F and x_D. (Luyben 1994).
- "Balanced structure I" (with varying reactor holdup): Control of x_r (reactor composition) and x_D. (Wu and Yu 1996).
- "Balanced structure II" (with varying reactor holdup): Control of F/F_0 and x_D. (Wu and Yu 1996).
- "Luyben's rule"(D or F) (Luyben 1993*b*) applied to case with constant reactor holdup: Control of M_r and D or F (structures CD or CF in Wu and Yu (1996)).
- "Reflux ratio" (L/F): Control of M_r and L/F (this paper).

Here Luyben's structure (LS) and the balanced structures are "unconventional" in the sense that the reactor level is left floating, which may at first may seem impossible. However, the reactor level has a steady-state effect through its effect on the conversion, and will therefore be indirectly given by specifying some other variable, for example, x_r or F (If desired, for example for safety reasons, one may install a reactor level controller as an inner cascade, with the level setpoint replacing the flow used for level control as a degree of freedom. This will *not* affect the steady-state behavior).

The above works raise some issues that needs to be studied further. First, in most of the above works, the overall operational objectives for the plant were not clearly defined. Second, a liquid phase reactor should normally be operated at maximum holdup (liquid level) in order to optimize steady-state economics, whereas the reactor level floats in the "unconventional" structures of Wu and Yu (1996) and Luyben. This has an impact on the steady state economics, an issue that has been overlooked by most researchers so far. Third, "Luyben's rule" of controlling a flow in the recycle loop (D or F) has not been properly substantiated. To the contrary, Wu and Yu (1996) found that the "Luyben structure" (LS) resulted in snowballing in the reactor holdup, and that "Luyben's rule with constant reactor holdup" (D or F) could handle only very small throughput changes.

The objective of this paper is to study in a systematic manner the selection of controlled variables for the reactor with recycle process. To this end we will use the general procedure of Skogestad (2000), where we first define the economic and operational control objectives and identify the available degrees of freedom. *The goal is to find a self-optimizing control structure where acceptable operation under all conditions is achieved with constant setpoints for the controlled variables.* However, before describing this procedure and applying it to the case study, we discuss in some more detail the socalled snowball effect.

Plant data. The plant and design data are taken from Wu and Yu (1996). The model is simple and assumes a binary feed ($x_0 = 0.9$ mol A/mol and $F_0 = 460$ kmol/h), isothermal reactor with maximum holdup 2800 kmol, and a first-order reaction $A \rightarrow B$ with $k = 0.341\ \text{h}^{-1}$. The distillation column has 22 stages including reboiler and condenser, liquid feed at stage 13, constant relative volatility $\alpha_{AB} = 2$, and constant molar flows. The purity requirement for the product is $x_B \leq 0.0105$ mol A/mol. From the total mass balance of component A, the nominal reactor concentration is

$$x_r = \frac{F_0(x_0 - x_B)}{kM_r} = \frac{460(0.9 - 0.0105)}{0.341 \cdot 2800} = 0.43 \tag{1}$$

2 The snowball effect

Luyben (1993*a*) introduced the term "snowball effect" to describe what can happen, for the recycle process in Figure 1, in response to an increase in the fresh feedrate F_0. For our process, where all the feed is converted to the product, the increase in F_0 must be accomponied by a corresponding increase in the conversion in the reactor. Assume that we in Figure 1 have a liquid phase CSTR with a first-order reaction. The amount of A converted in the reactor is then

$$kM_r x_r \quad [\text{molA/s}]$$

We see that there are three options for increasing the conversion (Wu and Yu 1996):

1. Increase the reaction constant k [1/s] (e.g. by increasing the reactor temperature)
2. Increase the reactor holdup M_r [mol]
3. Increase the reactor mole fraction x_r [mol A/mol] of reactant A

We assume here that option 1 (incrasing k) is not available.

Option 2 (increasing the reactor holdup) is probably the "default" way of dealing with a feedrate increase when seen from a design person's point of view. More specifically, a design person would increase all extensive variables (including flows) in the process proportionally to F_0, such that the intensive variables (compositions) in the process were kept constant. This is also the idea behind the "balanced" control structures of Wu and Yu (1996). However, changing the reactor holdup (volume) during operation may not be possible, or at least not desirable since for most reactions it is economically optimal to use a fixed *maximum* reactor volume in order to maximize per pass conversion.

Assuming k and M_r constant, the only remaining way to increase conversion is to follow option 3 and increase x_r, which can be done by recycling more unreacted A. However, the effect of this is limited, and the snowball effect occurs because even with infinite recycle D the reactor concentration cannot exceed that of pure A ($x_r = 1$). More precisely, for the process in Figure 1 the material balance equations for component A and total mass are (Luyben 1994)

$$\text{Overall process}: \quad F_0 x_0 = B x_B - k M_r x_r; \quad F_0 = B$$

$$\text{Column}: \quad F x_r = B x_B + D x_D; \quad F = B + D$$

Here x_0, x_D and x_B denote the mole fractions of component A in streams F_0, D and B, respectively. By eliminating x_r we find:

$$F = F_0 \, \frac{k M_r (x_D - x_B)}{k M_r x_D - F_0 (x_0 - x_B)} \tag{2}$$

If the reactor holdup is large relative to the feedrate, then we have almost complete conversion in one reactor pass and no recycle, so $D \approx 0$ and $F \approx F_0$, that is, the column feedrate F increases linearly with the fresh feedrate F_0. For larger values of F_0, the denominator in (2) will approach zero (and x_r will approach x_D), and we will experience "snowballing" with very large increases in D and F in response to only moderate increases in F_0. If the reactor holdup is too small compared to F_0, that is if

$$M_r \leq \frac{F_0 (x_0 - x_B)}{k x_D} \tag{3}$$

then the desired steady-state is infeasible (even with infinite flow rates for D and F). In practice, because of constraints, the flow rates will not go to infinity. Most likely, the liquid or vapor rate in the column will reach its maximum value, and the observed result of snowballing will be a breakthrough of component A in the bottom product, that is, we will find that we are not able to maintain the product purity specification (x_B).

To avoid this snowballing, Luyben et al. and Wu and Yu (1996) propose to use a varying reactor holdup (option 2), rather than the "conventional" control structure with constant holdup (option 3). Their simulations confirm that a variable holdup results in less snowballing in D and F, but these simulations are misleading, because they do not consider the reactor holdup. In fact, the Luyben structure (LS), with fixed D or F, may result in snowballing in the reactor holdup (Wu and Yu 1996). This is confirmed by Figure 2, where we see that that an increase in the feedrate may result in:

- Conventional structure (constant x_D) with constant reactor holdup: Snowballing in recycle flow (this is the snowballing considered by Luyben)

- Luyben structure (LS) with varying reactor holdup: Snowballing in reactor holdup

- Luyben rule (constant D or F) with constant reactor holdup: Snowballing inside column

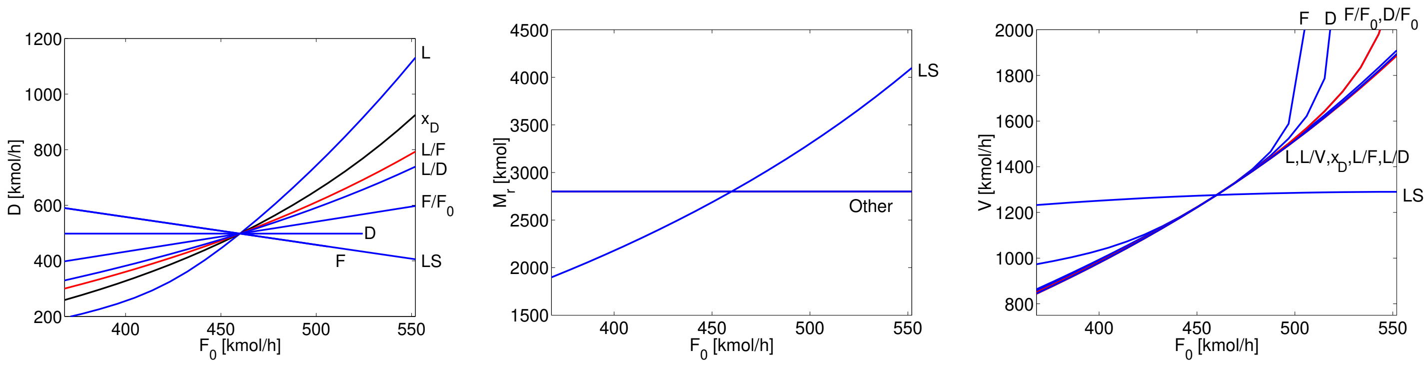

Figure 2: Snowballing: Steady-state values of the recycle flow (D), reactor holdup (M_r) and column boilup (V) as a function of feedrate F_0 for alternative control structures.

Actually, the snowballing in the recycle flow with the conventional structure is not as even as poor as shown in Figure 2. This is because we here used an intermediate value for the constant reactor holdup ($M_r = 2800$ kmol), whereas from (2) we find that the lowest value of F for a given value of F_0 is when the reactor holdup M_r is at its maximum – so with a fixed *maximum* holdup the conventional structure (x_D) actually gives smaller flows (D and F) than the Luyben structure (LS) in all cases.

In summary, the "snowball effect" is a real operational problem if the reactor (or some other unit in the recycle loop) is "too small", such that we may get close to or even encounter cases where the feedrate is larger than the reactor (or rather the system) can handle. The "snowball effect" makes control more difficult and critical, but it is not a control problem in the sense it can be avoided by use of control. Rather, it is a design problem which could have been be avoided by installing a sufficiently large reactor to begin with. In conclusion, for an existing plant the best remedy against snowballing is to use the maximum reactor holdup.

3 General procedure for selecting controlled variables

A plant generally has several operational degrees of freedom (manipulated variables) (there are six for our recycle plant, see Table 2). The objective of the control system is to adjust these manipulated variables to assist in achieving acceptable operation of the plant. Thus, to design a control system in a systematic manner we first need to define the operational requirements (constraints) and the goal of the operation. In general, we have upper and lower constraints on all extensive variables in a process, and on many intensive variables. The goal of the operation is quantified by defining a scalar cost function J to be minimized. The optimum (minimum value of J) usually lies at some constraints, and usually most of the degrees of freedom are consumed to satisfy these "active" constraints. However, in many cases there are unconstrained degrees of freedom, and the difficult issue is to decide what to control (that is, what to keep at a constant setpoint) in order to satisfy these. If we used optimal setpoints and there were no uncertainty or disturbances, then this choice would not matter. However, there will always be uncertainty and disturbances, and the optimal setpoints for the controlled variables should be insensitive to such changes. In addition, the shape of the objective function should be "flat", so that an implementation error will give a small loss (Skogestad 2000). To address this is a systematic manner, we will consider the economic loss imposed by keeping a given set of variables constant.

We assume that J is the economic cost, determined mainly by the plant's steady-state behavior, and from Skogestad (2000) adopt the following procedure for selecting the controlled variables:

Step 1: Degree of freedom analysis. Determine the degrees of freedom available for steady-state optimization. The easiest way is to count the number of manipulated variables and subtract the number of variables with no steady state that need to be controlled (e.g. reboiler and condenser levels in distillation).

Step 2: Cost function and constraints. Define the optimal operation problem by formulating a scalar cost function J to be minimized, and specify the constraints.

Step 3: Identify the important disturbances. Here "disturbances" include process disturbances, implementation errors in the controlled variables (sum of steady-state control error and measurement noise), as well as the effect of changes and errors (uncertainty) in the model.

Step 4: Optimization. The steady-state optimization problem is solved both for the nominal case and for the identified range of disturbances.

Step 5: Identify candidate controlled variables c. Active constraints should normally be controlled, as this optimizes steady-state cost. To select between the remaining unconstrained candidates we proceed to step 6.

Step 6: Evaluation of loss. Evaluate the loss for alternative sets of controlled variables c. Here the loss is the difference between the cost with constant setpoints c_s and the theoretical optimal cost (with setpoints reoptimized for each disturbance d),

$$L = J(c_s, d) - J_{\text{opt}}(d) \tag{4}$$

"Self-optimizing" controlled variables c with a small loss L are preferred.

Step 7: Further analysis. Normally several candidates gives an acceptable loss, and further analysis may be based on a controllability analysis.

4 Selection of controlled variables for the recycle plant

In this section, we use the concept of self-optimizing control, introduced above, to select the controlled variables for the recycle plant. To quantify the goals of operation, we define a scalar economic cost function J to be minimized, or equivalently, a profit function P [\$/s] to be maximized. We here select P [\$/h] as the difference between the value of the product B and the feed F_0, and subtract the operational costs for distillation and recycling:

$$P = -J = p_{F_0} F_0 - p_V V - p_D D \tag{5}$$

Here p_{F_0} [\$/mol] is the difference between the product and feedstock prices and we have used $B = F_0$. $p_V V$ is the energy cost related to distillation (since the column has a liquid feed and total condenser, the vapor flows to be evaporated and condensed are approximately the same, and p_V [\$/mol] is the sum of the price for reboiling and condensing). The recycle cost $p_D D$ may include costs for pumping and preprocessing (e.g. heating) the stream D. This cost is here neglected, but for gas phase systems with compression the term is usually important.

In general, the optimal way of operating the plant depends on the relative prices. However, for our problem the following two constraints are always active:

- Since the product (mostly B) is more valuable than the feedstock (mostly A), it is optimal to put as much unreacted A into the product as possible, that is, it is always economically optimal to operate with the bottom purity at its constraint (i.e. $x_B = 0.0105$).

- Since there is no economic penalty involved in increasing the reactor holdup, it is optimal for this reaction to keep M_r at its upper bound (i.e., $M_r = 2800$). This maximizes conversion "per pass", which reduces recycle and thereby the load on the distillation column.

We will in the following consider two different cases:

Case I: Given feedrate. With F_0 given and negligible recycling costs ($p_D = 0$), the profit P is only influenced by the energy costs $p_V V$ for heating and cooling in the distillation column. Thus, with a given feedrate F_0, optimal operation is obtained by minimizing the boilup V.

Case II: Variable feedrate. With F_0 as an unconstrained degree of freedom, we find that it is optimal to incease the feedrate F_0 as much as possible (since the profit P increases linearly with F_0 when we increase all other flows in proportion to F_0). However, there are always capacity constraints, and we assume here that the first one to become active is the vapor flow constraint $V \leq V_{max}$ in the distillation column. With $V = V_{max}$ and negligible recycling costs, the profit P is only influenced by the feedrate F_0. Thus, with variable feedrate, optimal operation is obtained by maximizing the feedrate (and production rate) F_0.

All the results in this section are based on a steady-state analysis. Table 1 summarizes the results which are further discussed below.

4.1 Case I: Given feedrate, minimize operation cost (energy)

Step 1: Degree of freedom analysis. From Table 2 we see that there are 4 degrees of freedom at steady-state, including F_0.

Step 2: Cost function and constraints. As noted above the objective is to minimize the vapor boilup, i.e. $J = V$. There are constraints on the reactor holdup (M_r), product quality (x_B) and column capacity (boilup V). In addition the feedrate F_0 is given.

Step 3: Disturbances. The main disturbance is in the feedrate F_0, and we consider $\pm 20\%$ changes. We also consider disturbances in the feed composition, $x_0 = 0.9 \pm 0.1$, but these turn out to be of much less importance. The implementation error is assumed to be $\pm 20\%$ in each of the candidate variables, and we also consider a ± 0.002 implementation error (possibly caused by poor dynamic control) in the product composition x_B. (Other possible disturbances, not considered here, include a change in the reaction rate constant k, and a change in the reactor holdup M_r).

Step 4: Optimization. Table 3 shows the results of the nominal optimization. As expected, the two constraints on x_B and M_r are active. Since the feedrate F_0 is given, we are then left with one unconstrained degree of freedom.

Step 5: Candidates for control. We choose to control the active constraints in order to optimize operation, i.e. M_r and x_B are controlled. This rules out the "unconventional" structures with variable reactor holdup, including the "Luyben structure" and the "Balanced structures".

Some of the candidates for the remaining degree of freedom are listed in Table 1. Two candidate variables have already been eliminated:

- The reactor composition x_r cannot be specified independently and is thus not a candidate for control. This follows from (1), since the feed is given (F_0 and x_0) and x_B and M_r are controlled at their constraints.

	Case I: Min. operation cost (energy)		Case II: Max. production rate	
Step 1: Degree of freedom analysis (see Table 2)				
	Degrees of freedom at steady state	4	Degrees of freedom at steady state	4
Step 2: Cost data				
	Objective function		Objective function	
	minimize V		maximize F_0	
	Constraints		Constraints	
	Reactor level $M_r \leq 2800$		Reactor level $M_r \leq 2800$	
	Product quality $x_B \leq 0.0105$		Product quality $x_B \leq 0.0105$	
	Feedrate $F_0 = F_{0,max} = 460$		Vapor boilup $V \leq V_{max} = 1500$	
Step 3: Identify most important disturbances				
	Disturbances		Disturbances	
	Feedrate $F_{0,max} \pm 20\%$		Maximum vapor boilup $V_{max} \pm 20\%$	
	Implementation error $\pm 20\%$		Implementation error $\pm 20\%$	
Step 4: Optimization				
-	Active constraints at the optimum	3	Active constraints at the optimum	3
	M_r, x_B, F_0		M_r, x_B, V	
=	Unconstrained degrees of freedom	1	Unconstrained degrees of freedom	1
	Nominal optimum: V=1276		Nominal optimum: F_0=497.8	
Step 5: Identify candidate controlled variables for unconstrained DOF (c)				
	F, L, D, $\frac{L}{D}$, $\frac{L}{F}$, $\frac{L}{V}$, x_D, $\frac{F}{F_0}$, $\frac{D}{F_0}$		F, L, D, $\frac{L}{D}$, $\frac{L}{F}$, $\frac{L}{V}$, x_D, $\frac{F}{F_0}$, $\frac{D}{F_0}$	
Step 6: Evaluation of loss with constant nominal setpoint, $c = c_s$)				
	Good candidates		Good candidates	
	x_D, L/F, L/D		x_D, L/F, L/D	
	Poor candidates		Poor candidates	
	F, D, L, F/F_0, D/F_0, L/V		F, D, L, F/F_0, D/F_0, L/V	
Step 7: Further analysis.				
	Ratio control (L/F or L/D) is easier than composition control (x_D).			
Conclusion				
	Control $\frac{L}{F}$ or $\frac{L}{D}$ (+ active constraints M_r, x_B, F_0)		Control $\frac{L}{F}$ or $\frac{L}{D}$ (+ active constraint M_r, x_B, V)	

Table 1: Summary of self optimizing control analysis.

	Manipulable variables	6
	Product flow B	
	Vapor boilup V	
	Reflux L	
	Recycle (distillate) D	
	Reactor effluent F	
	Feed F_0	
-	Controlled variables with no steady state effect	2
	Condenser level M_D	
	Boiler level M_B	
=	Degrees of freedom at steady state	4

Table 2: Degrees of freedom analysis.

	Case I: Min. V	Case II: Max. F_0	
Feedrate F_0	460	497.8	[kmol/h]
Reactor effluent F	958	1113	[kmol/h]
Vapor boilup V	1276	1500	[kmol/h]
Reflux L	778	885	[kmol/h]
Recycle (distillate) D	497	615	[kmol/h]
Recycle composition x_D	0.82	0.83	[mol A/mol]
Bottom composition x_B	0.0105	0.0105	[mol A/mol]
Reactor composition x_r	0.43	0.46	[mol A/mol]
Reactor holdup M_r	2800	2800	[kmol]

Table 3: Nominal optimization results for the two cases.

- The boilup V in the column is not a candidate for control as specifying it below its minimum (optimum) value results in infeasible operation.

Step 6: Evaluation of the loss. Figure 3 shows the loss in energy (i.e., increase in boilup V) imposed by keeping alternative controlled variables fixed at their nominal setpoints. The losses due to implementation errors (third row) and disturbances in F_0 (first row) are quite large for some variables. For example, we see from the first row that with L constant (left plot) a decrease in feedrate by 10%, results in using about 5% more energy than the optimal; this is reduced to less than 0.1% if we keep x_D constant and less than 0.01% if we keep L/F constant (right plot). The disturbances in feed composition x_0 (second row plots) result in very small losses in all cases. The loss due to a back-off in bottom composition from 0.0105 to 0.0085 is about 3% for all structures (last row).

In summary, Figure 3 shows that control of x_D, L/F or L/D give small losses (right plots), while control of F, D, L, L/V, F/F_0 or D/F_0 give large losses (left plots). In particular, we find that Luyben's rule of fixing one flow in every recycle loop, corresponding to fixing D or F, results in very large losses and even infeasibility, because V goes to infinity when F_0 increases (left plot in second row).

Step 7: Other considerations. The conventional control configuration with maximum reactor holdup (M_r), constant product composition x_B and constant setpoint for the distillate composition

(x_D) has very good self-optimizing properties with small economic losses. However, it may be costly to obtain on-line measurements of x_D, and two-point distillation composition control (of x_D and x_B) is known to be a difficult control problem due to interactions. In any case, the analysis shows that control of the internal distillate composition x_D is not really needed, since in terms of economic loss, control of L/F (or L/D) performs almost equally well. The latter results in a simple control problem and is therefore preferred. Figure 4 shows a possible control structure involving the following single loops: $M_r \leftrightarrow F$, $L/F \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

4.2 Case II: Maximize the feedrate

We now consider the case where the feedrate is a degree of freedom and should be maximized. This case is of more practical importance, since small losses in production rate usually have a large impact on overall plant economics.

Step 1: Degree of freedom analysis. As before, there are four degrees of freedom at steady state, see Table 2.

Step 2: Cost function and constraints. The goal here is to maximize the production rate, i.e. to minimize $J = -F_0$, and there are constraints on vapor boilup, reactor holdup and product composition.

Step 3: Disturbances. The main disturbance is in the actual value of the (maximum) boilup V_{max}, which may vary, for example, due to variations in the column pressure or available heat to the column.

Step 4: Optimization. Table 3 shows the results from the nominal optimization. We find as expected that all three constraints are active, including the maximum constraint on the vapor boilup. This leaves one unconstrained degree of freedom.

To understand why the production rate is limited, consider Figure 5. At low production rates (F_0) there is almost a linear relation between D and F_0. But as F_0 is increased, the load to the distillation column increases ($F = F_0 + D$ increases), and since $V = V_{max}$ is constant we eventually experience "snowballing" with breakthrough of product B in the top of the column. This results in a decrease (rather than the desired increase) in the fraction x_r of A in the reactor, and the production rate drops. This happens at $F_0 = 492.6$ kmol/h (the optimal point).

Step 5: Candidates for control. We consider the same candidate variables as in case I.

Step 6: Evaluation of the loss. Figure 6 shows the loss in production rate due to a disturbance in V and due to implementation error. Although the details are different, the results are similar to case I, with small losses for control of x_D, L/F and L/D.

Step 7: Other considerations. Again, since controlling L/F or L/D gives a much easier control problem for the distillation column it will be preferred over control of x_D. A possible control structure is shown in Figure 7. To be able to handle also case I, we have included is a cascade flow control loop where we obtain $F_0 = F_{0,s}$ by adjusting V, but this flow control (FC) loop is not used in case II where we have maximum vapor boilup ($V = V_{max}$).

Comment: The same variable, L/F or L/D, turned out to be a good unconstrained controlled variable for both cases I and II. This is generally attractive, as it may reduce the effort in reconfiguring the loops when, for example, the economic conditions change from case I (given production) to case II (maximize production).

5 Closed-loop simulations

In Figure 8 we show for case I (given feedrate F_0, no capacity limit on V) the closed-loop dynamic responses in bottom composition to a 20% increase in feedrate F_0 for the following structures:

Conventional (x_D) : $M_r \leftrightarrow F$, $x_D \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

Reflux ratio (L/F) : $M_r \leftrightarrow F$, $L/F \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

Luyben rule (F) : $M_r \leftrightarrow D$, F constant, $x_B \leftrightarrow V$, $M_D \leftrightarrow L$ and $M_B \leftrightarrow B$.

Luyben structure (LS) (varying reactor holdup): F constant, $x_D \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

Note that we have used single-loop controllers and $\leftrightarrow$ means "is paired with" or more precisely "is controlled by". The pairings are based on a relative gain array analysis, and PI-settings are found using the IMC-tuning approach. We selected 0.25 min as the desired closed-loop time constant for the level loops and 2.5 min for the other loops. For the three first structures we have constant maximum reactor holdup, $M_r = 2800$ kmol.

The conventional structure and reflux ratio structure yield very similar and acceptable dynamic responses.

The Luyben rule with constant F for the case with constant reactor holdup yields instability. It is not able to maintain the desired bottom composition even for small increases in the feedrate. This confirms the steady-state results in Figure 3 and the findings of Wu and Yu (1996). This is easily explained: As the feedrate F_0 is increased, we must with constant $F = F_0 + D$ reduce the recycle D to the reactor (which is the opposite of what we would like to do). This results in snowballing inside the distillation column with accumulation of unreacted component A, and operation eventually becomes infeasible.

The Luyben structure (LS) (with varying reactor holdup) clearly yields the best dynamic response in x_B; this is because the varying reactor holdup serves as a surge tanks which helps to smooth (average out) the feedrate disturbance. However, the response in x_B for the Luyben structure is unrealistic since we have allowed the reactor level M_r to exceed its maximum value, and we see from the right plot in Figure 8 that there is actually a snowballing in the reactor level (Wu and Yu 1996). To guarantee feasibility ($M_r \leq M_{r,max}$) for feedrate changes, we would for the Luyben structure need to "back away" from the reactor level constraint (using a nominal holdup significantly smaller than $M_{r,max}$), which would give non-optimal economic operation with about 50% higher energy usage (V) in the distillation column, or even worse, inability to handle the desired feedrate due to capacity limitations in the distillation column.

On the other hand, if we for the other structures (with constant holdup) introduce a back-off in bottom composition x_B from 0.0105 to 0.0085 (in order to handle the control variations in Figure 8) then the increase in energy usage (V) is only by about 3% (see lower plot in Figure 3). Alternatively, we may avoid the need for back-off in x_B (and the resulting 3% energy increase) by using a product tank with mixing to average out the dynamic variations in x_B.

6 Discussion

6.1 Alternative sets of active constraints

We have in this paper considered case I with a given feedrate and case II with an unconstrained feedrate, and these resulted in two different control structures. What other cases are there? We here define a "case" in terms of the set of active constraints. For our recycle plant the following four upper constraints are of interest:

$$x_B \leq x_{B,max}, \quad M_r \leq M_{r,max}, \quad F_0 \leq F_{0,max}, \quad V \leq V_{max}$$

Here, as explained earlier, the economic conditions are such that the two first constraints are always active, and at least one of the two latter constraints are active. We are then left with only three cases:

Case I : Constraint on $F_{0,max}$ is active and V is unconstrained. This happens for low values of the available feedrate $F_{0,max}$ (or large values of V_{max}), where it is optimal to process all the available feed while minimizing the value of V.

Case II : Constraint on V_{max} is active and F_0 is unconstrained. This happens for high values of $F_{0,max}$ (or low values of V_{max}), where the available feedrate $F_{0,max}$ exceeds the optimal maximum feedrate.

Case III : Constraints on $F_{0,max}$ and V_{max} are both active. This happens for intermediate values of the available feedrate $F_{0,max}$, provided there is some penalty on recycle, i.e. $p_D > 0$.

The details depend on the cost function $-J = p_{F_0}F_0 - p_V V - p_D D$. The feedrate range where case III is economically optimal is often quite small, especially if recycle costs are small compared to distillation costs. In this paper we have assumed no recycle costs ($p_D = 0$) and we go directly from case I to case II. For example, with $p_D = 0$ and $V_{max} = 1500$ [kmol/h], we have case I for $F_{0,max} \leq 468.6$ and case II for $F_{0,max} \geq 468.6$. With recycle costs included ($p_D > 0$) it is optimal to use more energy in the distillation column, and we get a region where both constraints are active (case III). For example, with the cost function $-J = F_0 - 0.01V - 0.1D$ (i.e., $p_{F_0} = 1, p_V = 0.01, p_D = 0.1$) and $V_{max} = 1500$, we have case I for $F_{0,max} \leq 468.6$, case III (both constraints active) for $468.6 \leq F_{0,max} \leq 493.2$, and case II for $F_{0,max} \geq 493.2$. Note here that the economic maximum capacity of 493.2 is somewhat less than the achievable maximum capacity of 497.8 [kmol/h].

In the above discussion we have considered the "available feedrate" $F_{0,max}$ (inequality constraint $F_0 \leq F_{0,max}$). For the closely related case with a "given feedrate" ($F_0 = F_{0,max}$) we have the following: At low feedrates F_0 we have case I with V unconstrained. As the feedrate increases, the boilup V also increases (the change in V for a small change in F_0 may be large if we experience snowballing), and eventually the column reaches its capacity limit (V_{max}). With constant boilup ($V = V_{max}$), it may be possible to increase the feedrate further by reducing the distillate purity x_D and increasing the recycle (case III) , but eventually the column becomes a bottleneck (case II) where it is not feasible to process any more feed while maintaining the given product composition.

Comment: The fact that the distillation column is a bottleneck in case II, does not necessarily mean that production rate can be much increased by increasing its capacity V_{max}, because if the system is close to snowballing, then increasing $M_{r,max}$ is the only effective way of increasing plant capacity.

6.2 Decentralized control and reconfiguration of loops

The focus in this paper is to decide on which variables to control, and we have recommended to use the "reflux ratio" structure with control of L/F. The analysis has been based on steady-state economics, and is independent of the actual implementation. However, in the closed-loop simulations we assumed decentralized control, where each controlled variable was paired with a manipulated input. A main problem with decentralized control is that reconfiguration of loops is generally required when the active constraints change. Let us consider this in more detail for our proposed reflux ratio structure.

We have already proposed pairings for cases I and II. In the intermediate case III there are no unconstrained degrees of freedom, that is, the economic optimal control structure is to use all four steady-state degrees of freedom to control the active constraints. A possible control structure for case III is then: $M_r \leftrightarrow F, x_B \leftrightarrow L, F_0 = F_{0,max}, V = V_{max}, M_D \leftrightarrow D$ and $M_V \leftrightarrow B$. Note that the reflux L is here used to control bottom composition. In summary, we then have for the "reflux ratio" structure (in all cases we use $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$):

$$\begin{array}{rllll} \text{Case I}: & M_r \leftrightarrow F & L/F \leftrightarrow L & F_0 = F_{0,max} & x_B \leftrightarrow V \\ \text{Case II}: & M_r \leftrightarrow F_0 & L/F \leftrightarrow L & V = V_{max} & x_B \leftrightarrow F \\ \text{Case III}: & M_r \leftrightarrow F & F_0 = F_{0,max} & V = V_{max} & x_B \leftrightarrow L \end{array}$$

We note that two loops (control of M_r and x_B) need to be reconfigured as we go from case I to case II. To minimize the need for reconfiguration we may use the inflow F_0 to control the reactor level in all cases (this corresponds to setting the production rate at the column bottleneck (V) in all cases). We then get the control structure in Figure 7:

$$\text{Case I}: \quad M_r \leftrightarrow F_0 \quad L/F \leftrightarrow L \quad F_0 \leftrightarrow V \quad x_B \leftrightarrow F$$

In this case no reconfiguration is required as we go between cases I and II. The disadvantage is that control of feedrate F_0 is indirect so F_0 will deviate from $F_{0,max}$ when the process is disturbed. However, if we have a storage tank for the feed then this does not matter as the variations will average out over time.

6.3 Multivariable constraint control (MPC)

To avoid the logic in reconfiguring loops when switching between cases I, II and III, one may use a multivariable controller with explicit handling of constraints (e.g. model predictive control, MPC) that "automatically" reconfigures the control tasks when the active constraints change. However, also here one needs to decide on what variables to setpoint control to satisfy the unconstrained degrees of freedom (cases I and II). Thus, our recommendation of controlling the reflux ratio (L/F) applies also to MPC.

The objective of the model predictive controller would then be to control x_B (first priority) and L/F (second priority) at their setpoints (and possibly also the reactor level, condenser level and reboiler level, but we assume these are controlled by a lower-layer level control system), using the degrees of freedom F_0, V and L (assuming here that F, D and B are used for level control in the lower layer), subject to given constraints on F_0 and V. The setpoints which may vary with time, are supplied by the layer above MPC. This may be a steady-state optimizer or an operator.

6.4 Economics not important

We have in this study excluded the "unconventional" control structures with variable reactor holdup (Luyben 1994) (Wu and Yu 1996) from being economically optimal. However, with a given feedrate

F_0, low energy and recycle costs (p_V and p_D small), and no capacity constraints (V_{max} large), the economic penalty of using $M_r < M_{r,max}$ may be small, and it may be more important to operate the plant as smoothly as possible, for example, to reduce the effect of disturbances on other parts of the plant. In such cases, a variable reactor holdup structure, such as one of the balanced structures of Wu and Yu (1996), may be better, because the reactor is effectively used as a surge tank to "average out" disturbances in the column feedrate. Nevertheless, we do *not* recommend the Luyben structure (LS) (Luyben 1994) with a fixed flow in the recycle loop, since it results in snowballing in the reactor holdup (Wu and Yu 1996); see also Figure 8. This is also explained since we in response to an increase in feedrate clearly should increase the recycle (and not keep it constant).

7 Conclusion

We have presented a systematic approach for selecting controlled variables for the liquid phase reactor with recycle plant. To optimize economics we need to control active constraints. Both for the cases of minimizing operating costs (case I) and maximizing production rate (case II), it is optimal to keep the reactor holdup at its maximum. This makes the Luyben structure (LS) and the two balanced structures of Wu and Yu (1996) economically unattractive. For the unconstrained variables we look for self-optimizing variables where constant setpoints give acceptable economic loss. Both in cases I and II, the reflux ratio (L/F or L/D) appears to be such a variable. In order to avoid the socalled "snowball" effect, it has been proposed in the literature to "fix a flow in a liquid recycle loop". However, the rule seems to have limited basis, as it leads to control structures that can handle only small feedrate changes (constant reactor holdup), or that result in large variations in the reactor holdup (variable reactor holdup) (Wu and Yu 1996).

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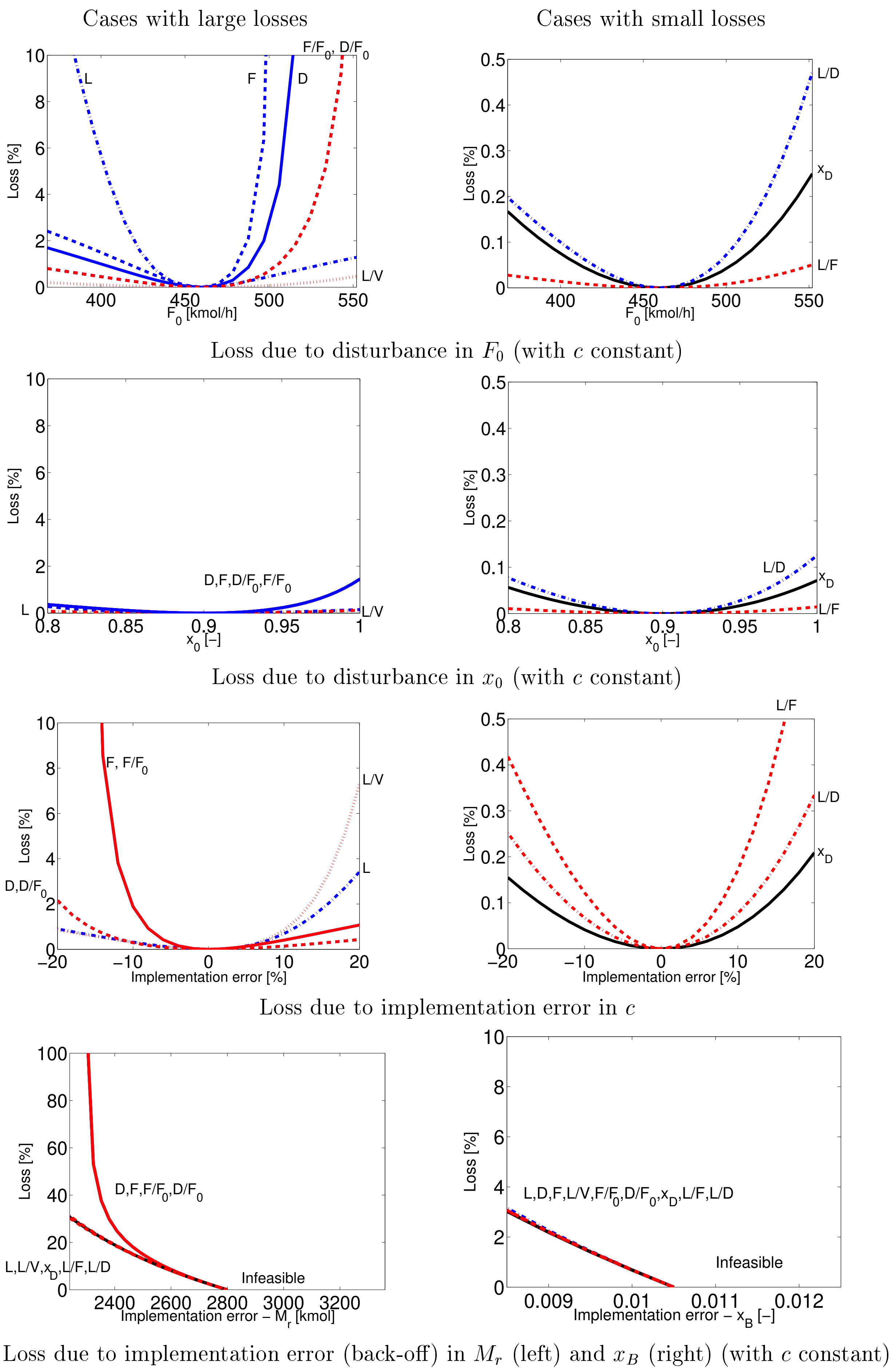


Figure 3: Case I: Losses in energy (V) with alternative controlled variables ($F_0 = 460, M_r = 2800, x_B = 0.0105$).

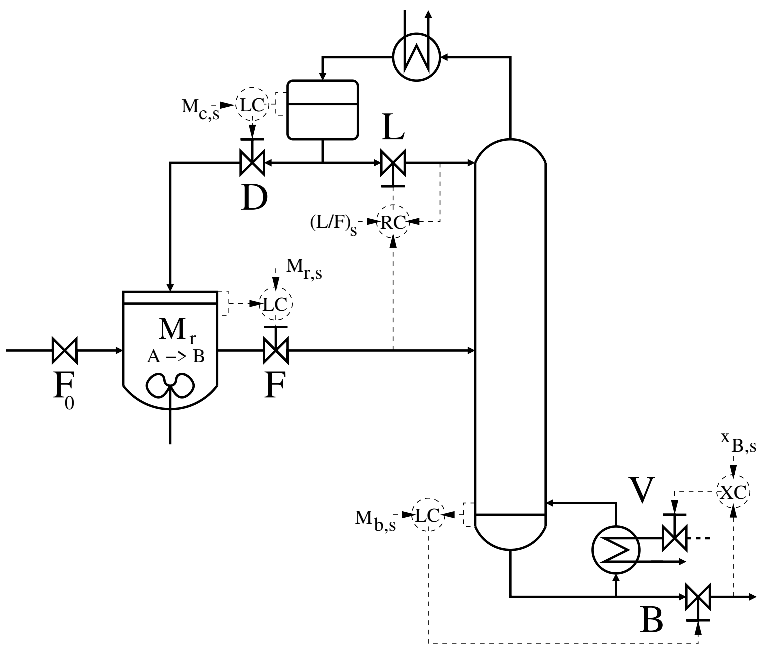


Figure 4: Reflux ratio control structure (Case I with given feedrate)

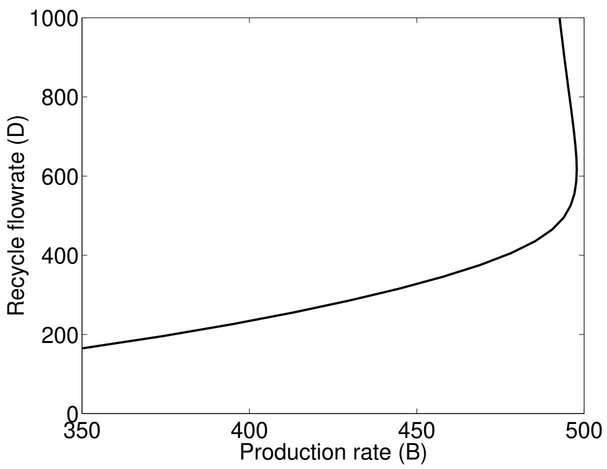
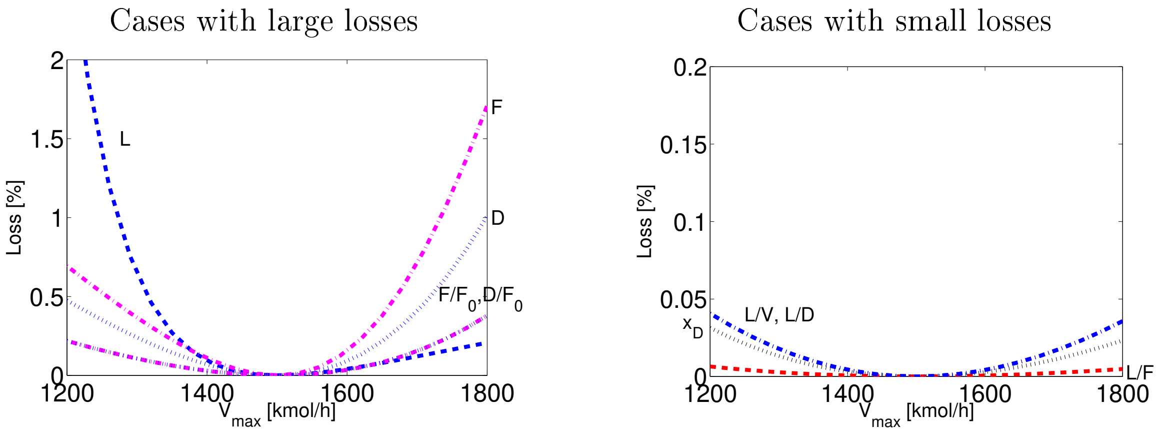
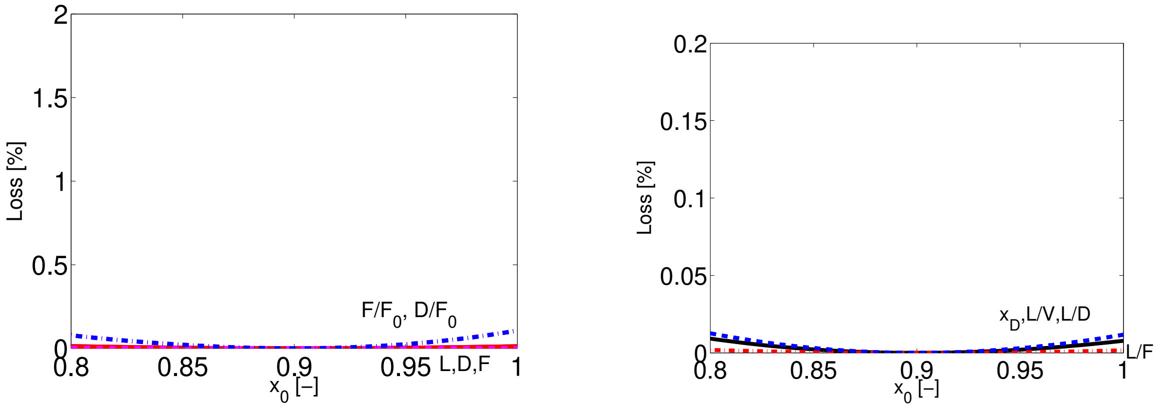


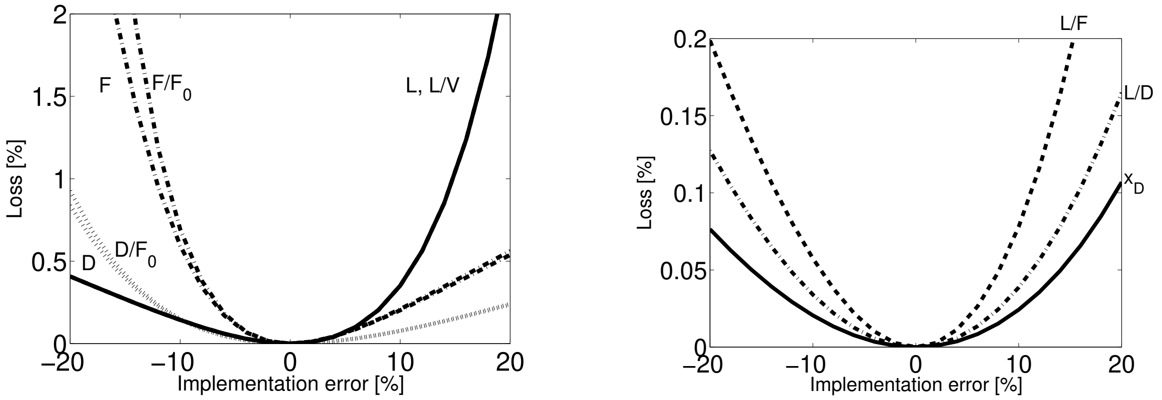
Figure 5: Snowballing with V constant: Recycle flow D as a function of production rate $B = F_0$ (Case II, $M_r = 2800$, $x_B = 0.0105$, $V = 1400$).



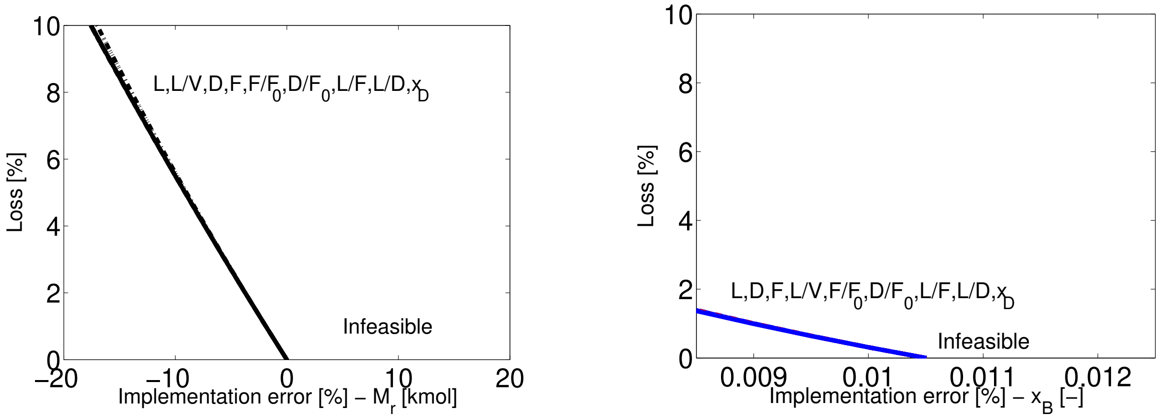
Loss due to disturbance in V (with c constant).



Loss due to disturbance in x_0 (with c constant).



Loss due to implementation error in c.



Loss due to implementation error (back-off) in M_r (left) and x_B (right) (with c constant).

Figure 6: Case II: Losses in production rate (F_0) for alternative controlled variables ($V = 1500, M_r = 2800, x_B = 0.0105$)

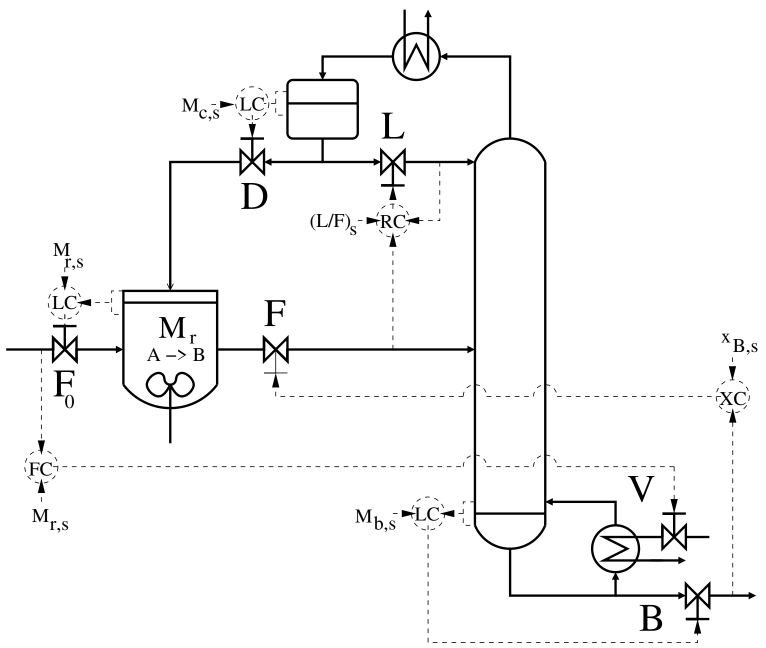


Figure 7: Reflux ratio control structure for case II (with flow control loop to handle also case I)

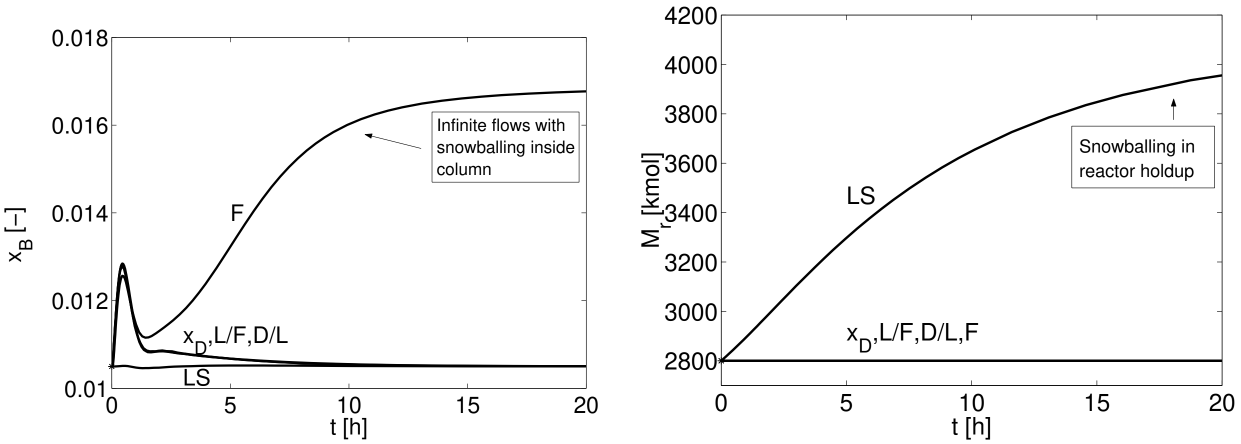


Figure 8: Dynamic responses in x_B (left) and M_r (right) to a 20% step increase in F_0 (Case I) for alternatice control structures

x_D : Conventional structure (constant x_D and M_r)

$D/L, L/F$:Reflux ratio structures (constant D/L or L/F and M_r)

F : Luyben rule for case with constant M_r (constant F and M_r)

LS : Luyben structure with varying reactor holdup (constant F and x_D)