Control of reactor, separator with recycle.

Liquid phase system
gas phase systems
methanol synthesis loop

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Motivation, background and related work

- Common feature of many chemical processes.
- Examples includes: Methanol synthesis loop, ammonia plants.
- Recycle changes the behavior of the plant: A plant-wide view is needed.
- Control of these plants has been studied extensively in the literature.
- A systematic framework for comparisons is needed.

The main issue: **selection of controlled variables**.

Will be based on the concept of self-optimizing control.

Which involves searching for the variables which when kept constant give the minimum operating costs, (Skogestad *et al.* 1999).

In this work we will study to simple cases

- a liquid phase reactor and
- a gas phase reactor (more common in the industry),

and a case based on

- methanol synthesis loop

Difference, and similarities between them will be discussed.
Conclusions are supported by simple models.

Related work

A lot has been on the control of liquid phase system.
Less has been done on gas phase systems.

- Gilliland *et al.* (1964): Showed how recycle increased gain and time constants for the whole system. Explained by positive feedback due to mass recycle.
- Papadourakis *et al.* (1987): The RGA for the individual units are different than the RGA of the whole plant. Recycle changes the interactions in the plant.
- Wolff *et al.* (1992): looked on the effect of recycle on the controllability.
- Price and Georgakis (1993): looks at simulation of a large number of control structures, from which they makes general guide lines.
- Luyben and Floudas (1994): look into the interactions between design and control using multi objective optimization.
- Luyben (1993a, 1993b, 1994): has studied several recycle process. As a remedy for the high gain in recycle flow he proposes to fix a flow in the recycle loop.
- Wu and Yu (1996): They show that for a fixed reactor effluent flow, the reactor hold-up has a high gain for feed-rate changes. Their solution is to distribute the load changes on different units.
- Fisher *et al.* (1988): must be mentioned here. On page 613 there is some heuristics for plant control. One such heuristics is: "keep the gas recycle flow at its maximum value". They advocates to keep the recycle flow at its maximum value in order to increase the yield. They used the HDA as an example.
- (Hansen 1998). He presents a interesting controllability analysis of the methanol loop. The conclusion is that the design has good dynamic behavior. He is more unclear when he discusses the potential for optimizing control.

Simplified steady state equations

Sharp separation

Production rate

$$kM_r z = z_0 F_0$$

Given $F_0 \Rightarrow$ control either M_r or z.

Recycle as a function of reactor hold-up.

$$D = \frac{(F_0)^2}{kM_r - F_0}$$

Hold-up as a function of recycle

$$M_r = \frac{D + F_0}{D}\frac{F_0}{k}$$

To minimize recycle D, maximize reactor holdup M_r.

If there is inert present

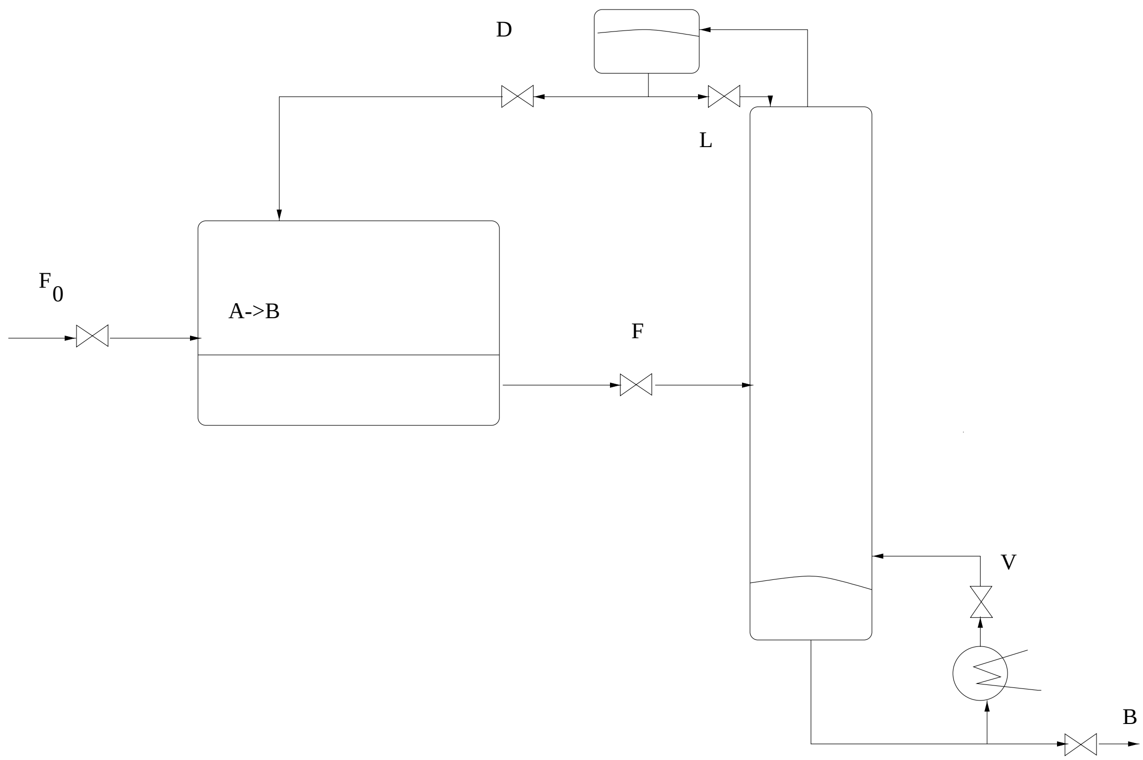
Minimum purge flow

$$S_{min} = \frac{F_0}{2} + \frac{kM_r}{2}\left(-1 + \sqrt{1 + \frac{2F_0(1-2z_0)}{kM_r} + \left(\frac{F_0}{kM_r}\right)^2}\right)$$

As $S \rightarrow S_{min}$ recycle goes to infinity.

S_{min} depends on reactor hold-up.

Economic analysis of the liquid phase system



Simple model:

First order kinetics $A \rightarrow B$ and reaction rate $kM_r z$.

No inerts, feed consist of A and B.

Constant temperature in the reactor.

Distillation column with constant relative volatility.

Have studied two different economic objective functions:

- Minimization of vapor boild-up, given feed rate.
- Maximization of production, feed rate is manipulative.

Maximization of production

Degrees of freedom analysis

Manipulative variables:	
Feed-rate F_0	1
Reactor effluent flow F	1
Recycle flow (distillate flow) D	1
Reflux L	1
Vapor boil-up V	1
Product flow B	1
Sum	6
Two levels without steady state effect	-2
Steady state degrees of freedom	**4**

Cost function and optimization

The goal is to maximize production

$$\begin{aligned} maximize \quad & F_0 \\ subject\ to \quad & M_r \leq 2800 \\ & x_B \leq .015 \\ & V \leq 1400 \end{aligned}$$

4 degrees of freedom at steady state, should be used to optimize

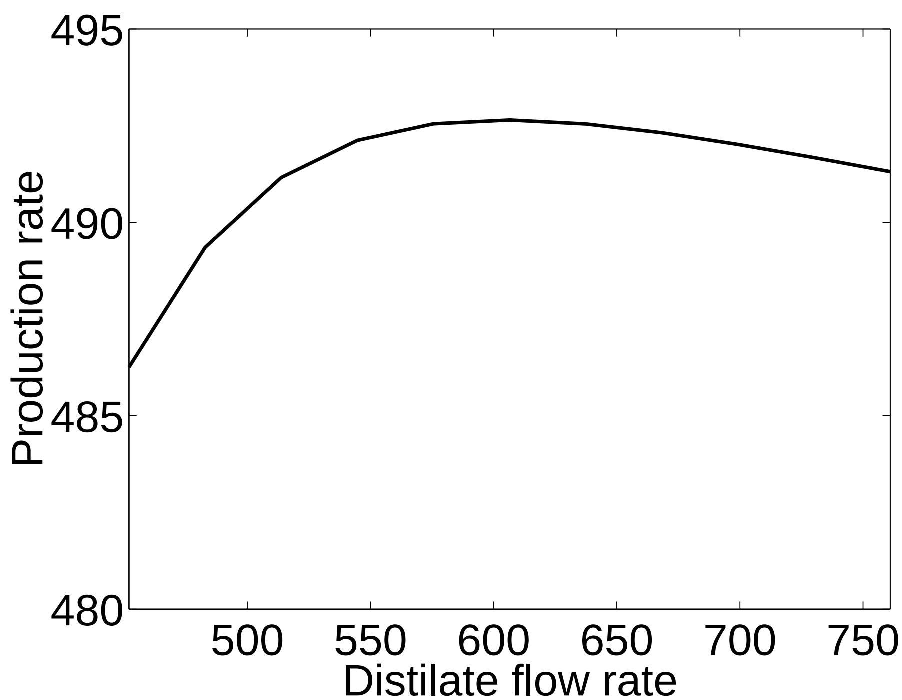
3 of these are constrained

x_B : Over purification of pruduct would waste a limited capacaty in the column.

M_r : There are no cost for increasing reactor level to its maximum value. But conversion will increase!

V : It is desirable to have as large recycle as possible, for any feed and feed composition this is achieved by increasing the vapor-boilup to its maximum value.

One unconstrained degree of freedom left.
How does our objective look like ?



$\pm 1\%$ for $\pm 20\%$ deviation from optimal recycle.

Thus a large error in implementing the optimal recycle rate, would only give a small deviation from maximum production.

Can we do better?

Disturbances

Max V ($\pm 20\%$).
Control error.

Candidates for controlled variables

D	Recycle flow rate
F	Reactor effluent flow rate
L	Reflux
L/F	Ratio of reflux and feed rate
L/D	Reflux ratio
x_D	Top composition

Evaluation of loss

Variable	Range		Max loss	
F	877 - 1315	kmol/s	16	
L	637 - 956	kmol/s	7	
L/F	0.581 - 0.872		1.3	
L/D	1.056 - 1.583		0.6	
x_D	0.795 - 0.835		0.1	*

Control of top composition gives the smallest loss.

But reflux ratio L/D could be preferred in practice.

Note Since we control M_r and $F_0 = kM_rz$. F_0 and z are not candidates as controlled variables.

Minimization of operation cost

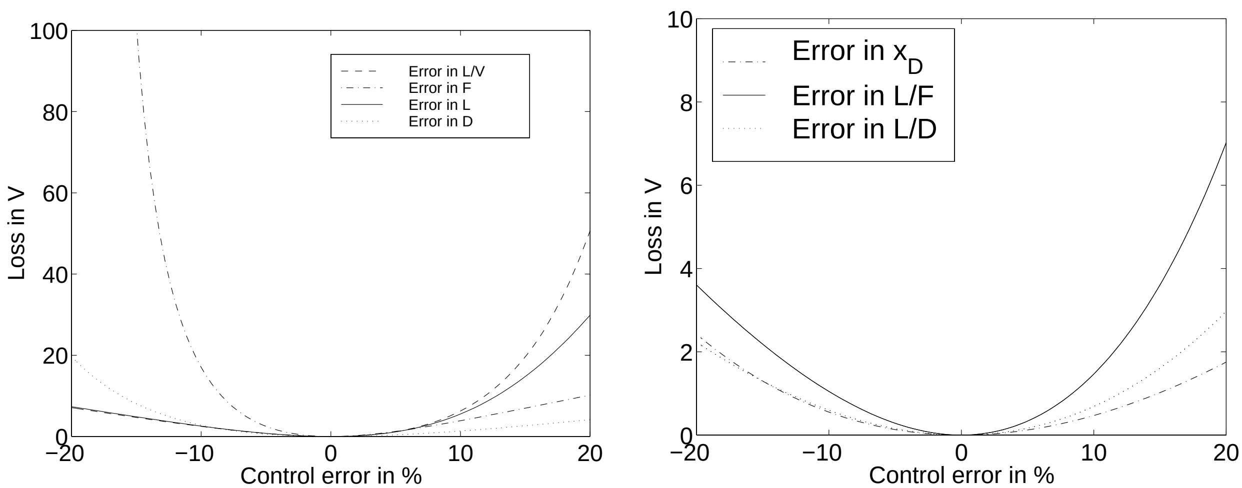
Operation costs related to vapor boil-up V.

$$\begin{aligned} minimize \quad & V \\ subject\ to \quad & f(x,u,d) = 0 \\ & M_r \leq 2800 \\ & x_B \leq .015 \end{aligned}$$

Different objective, different constraints, and feed rate is given.

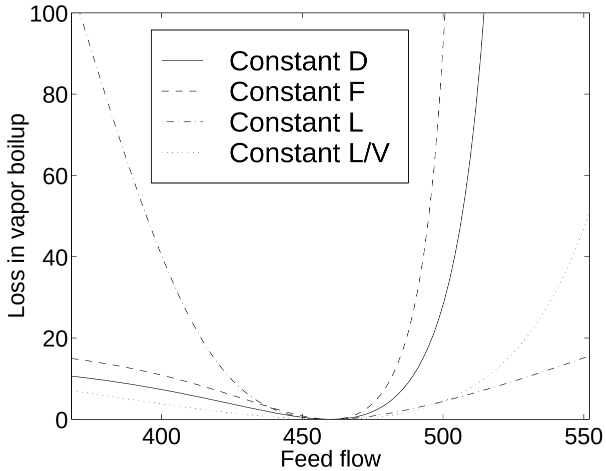
But: M_r and x_B are constrained
one unconstrained degree of freedom

Loss function for selected variables:

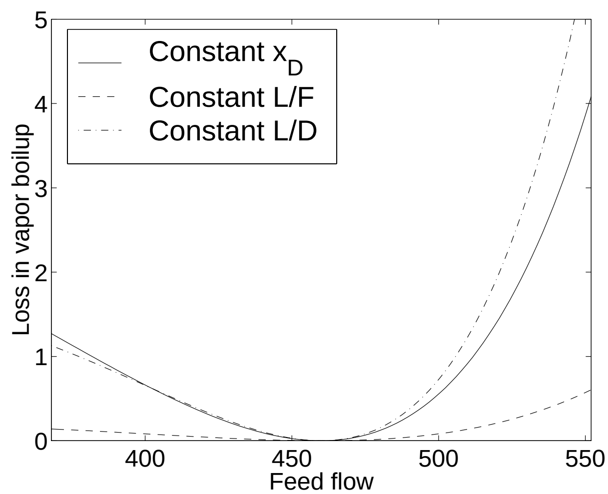


(a) Large losses (b) Small losses

Figure 1: Loss in vapor boil-up, for control errors in selected variables. The nominal values are $L/V = 0.59$, $F = 963$, $L = 713$, $L/F = 0.74$, $L/D = 1.42$ and $D = 503$. For x_D the range is from 0.76 to 0.84 (± 20 impurity)



(a) Large losses



(b) Small losses

Figure 2: Loss functions for keeping different variables constant. For all cases x_B and M_r are at the optimum value.

x_D, L/F or L/D: good candidates

The snowball effect?

Luyben (1994): “the use of a conventional control structure resulted in a 100% increase in the recycle flow rate for a 10% increase in the fresh feed flow rate. Such large changes are very undesirable because columns can only tolerate a limited turn-down ratio.”

His solution: fix the reactor effluent flow.

The high gain is illustrated by

$$D = \frac{F_0(F_0(z_0 - x_B) - kM_r x_B)}{kM_r x_D - F_0(z_0 - x_B)} \tag{1}$$

Small $M_r \Rightarrow$ high gain from F_0 to D.

The boil-up as a function of load changes

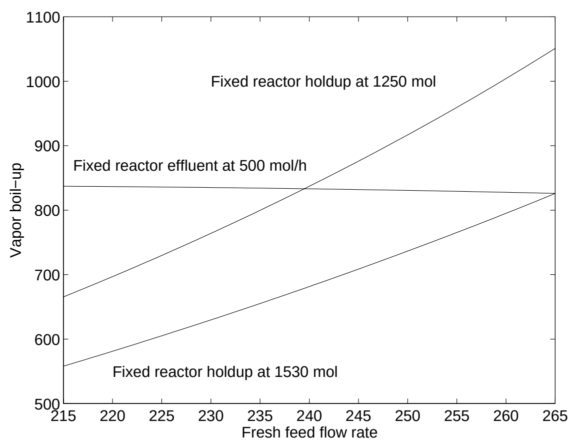


Figure 3: The steady state effect of load changes on boil-up.

- Fixed reactor effluent flow small variations in boil-up.
- Maximum reactor hold-up gave always lower boil-up.

Our solution:

1. Maximize reactor hold-up.

2. If necessary, put a lower limit on boil-up.

Controllability analysis

For the case with a given feed, let us study the controllability of some of the alternatives:

Case 1: Control of x_D, x_B and M_r.

Case 2: Control of L/F, x_B and M_r.

Case 3: Control of x_D, x_B and F.

Case 1 and case 2: good self-optimizing properties.
Case 3: We have applied the Luyben rule: "Fix one flow in recycle".

Is it possible not to control reactor level?

The pole direction gives us the answer:

```
y = -0.9907 xb   u = -0.4336  F
    -0.0206 xd        0.4621  D
     0.1348 Mr        0       L
     0      Mb        0       V
     0      Md        0       B
```

The "reactor level" can be stabilized by loops not involving M_r.

If we pair to avoid negative RGA at steady state, and RGA near one at crossover frequency, we get the following pairings:

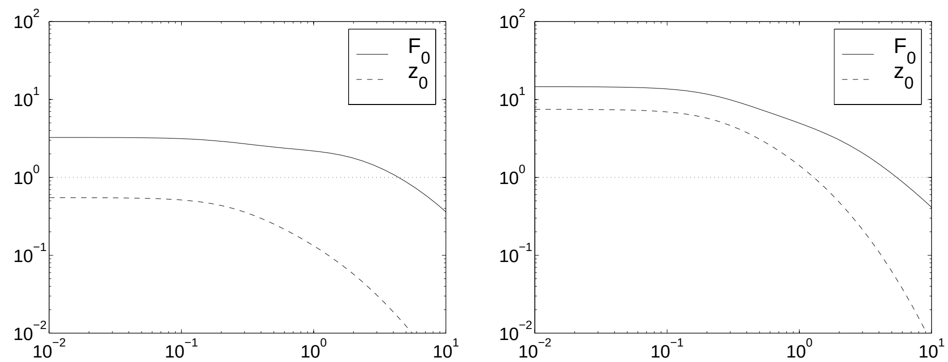
For case 1: $x_B - V$, $x_D - L$, $M_r - F$, $M_B - B$ and $M_D - D$.

For case 2: $x_B - V$, $M_r - F$, $M_B - B$ and $M_D - D$.

For case 3: $x_B - V$, $x_D - L$, $M_B - B$ and $M_D - D$.

Perfect level control, and we assume that the ratio is implemented as $L = \frac{k}{\tau s+1}F$.

We will look at closed loop disturbance gain, to see if any of the proposed control configurations has better disturbance rejection properties.



(a) Output x_D (b) Output x_B

Figure 4: Closed loop disturbance gain for case one.

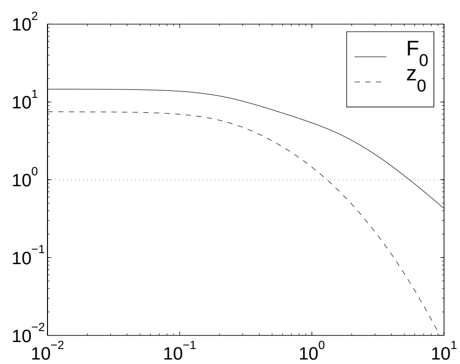
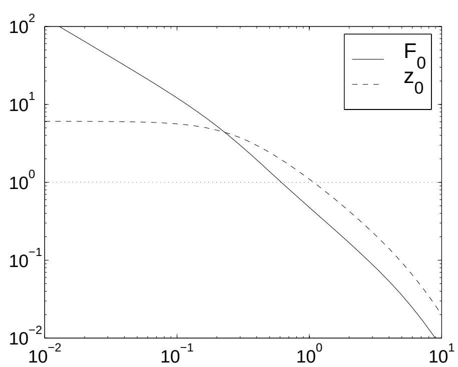
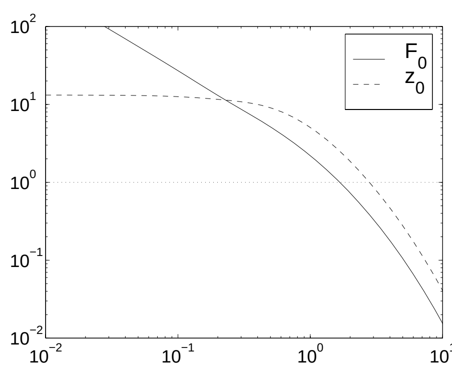


Figure 5: Disturbance gain for case 2.



(a) Output x_D

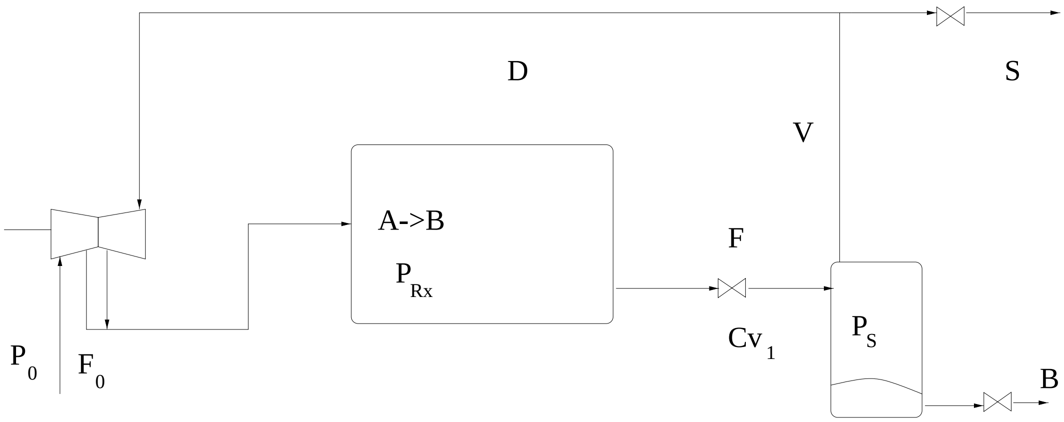


(b) Output x_B

Figure 6: Closed loop disturbance gain for case three.

Does not seem to be a large difference in controllability for the three alternatives.

Economic analysis of the gas phase system



Difference

- Perfect separation.
- Including inert.
- Cost of holdup : Compression cost.
- Cost of recycle : Compression cost.

Degrees of freedom analysis

Manipulative variables (given feed-rate):

Purge flow S	1
Flow control valve opening	1
Product flow	1
Sum	3
Level without steady state effect	-1
Minimize pressure drop	-1
Degree of freedom at steady state	1

Compressor work is not a degree of freedom if F_0 is given.

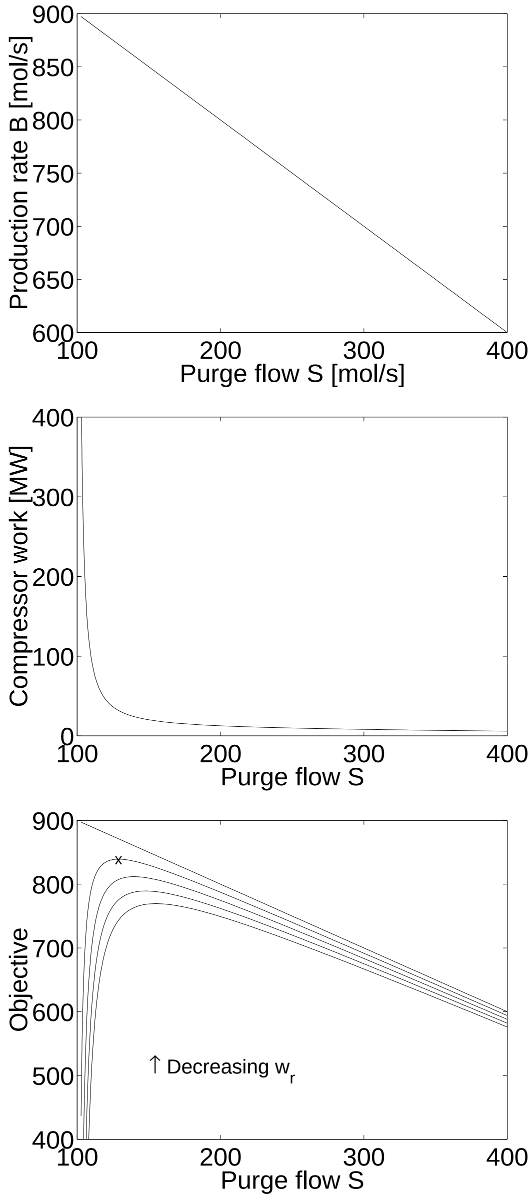
Cost function and optimization

The cost of operation is given by maximum production and compressor work

$$J = B - w_r\left(W_1 + W_2\right)$$

There is a cost associated with hold-up in the reactor P_r!

Optimization

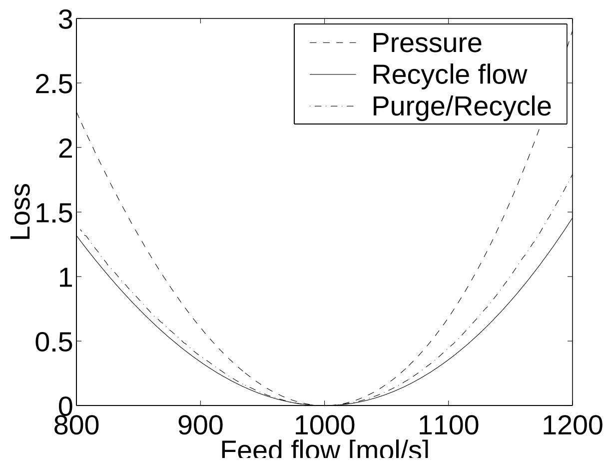


Candidates for controlled variables

Loss due to control error:

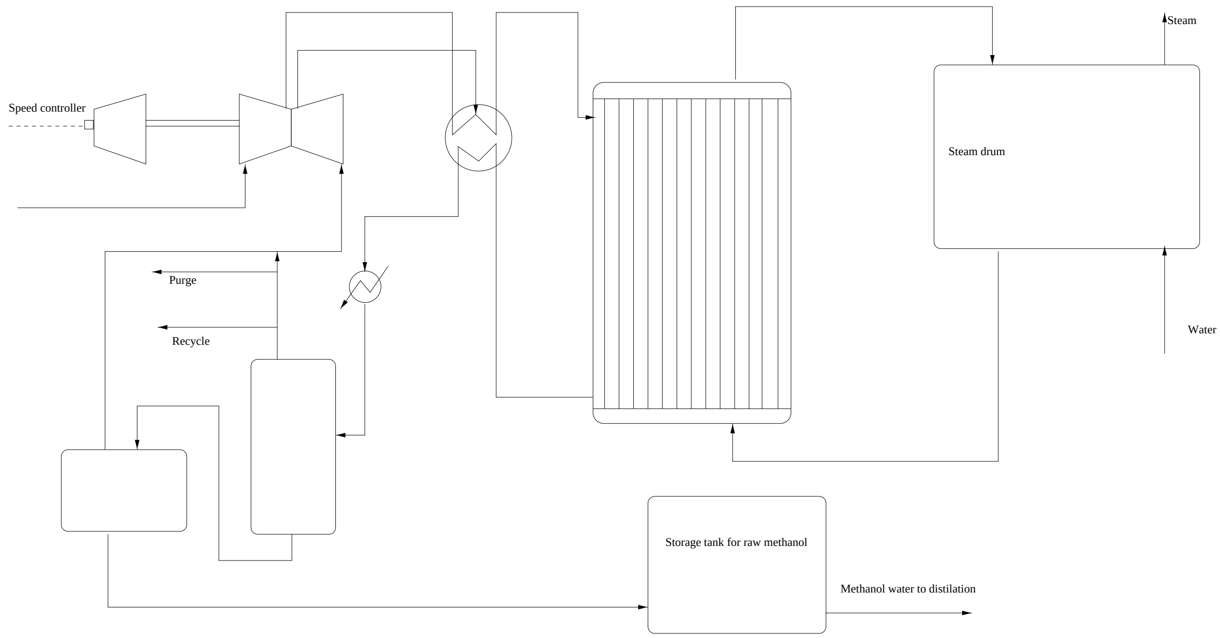
Variable	Range		Max. loss
S	103 - 155	mol/s	330
R	2230 - 3345	mol/s	1.7
S/R	0.037 - 0.055		1.2
z_I	0.676 - 0.876		18.2
P_{Rx}	189 - 231	bar	1.0

Loss due to distrubance:



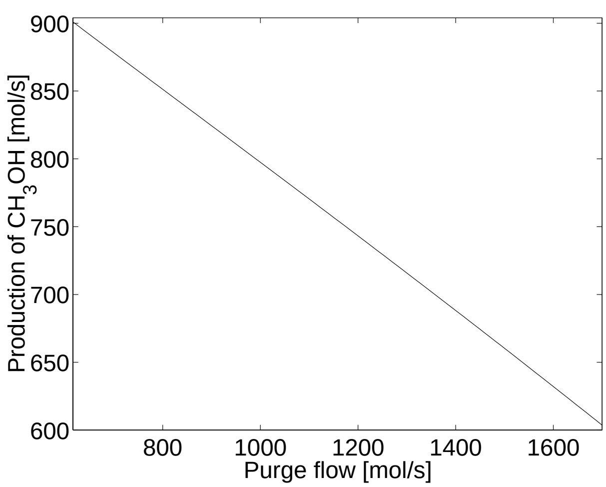
Control of R, P_{rx} or S/R are good alternatives

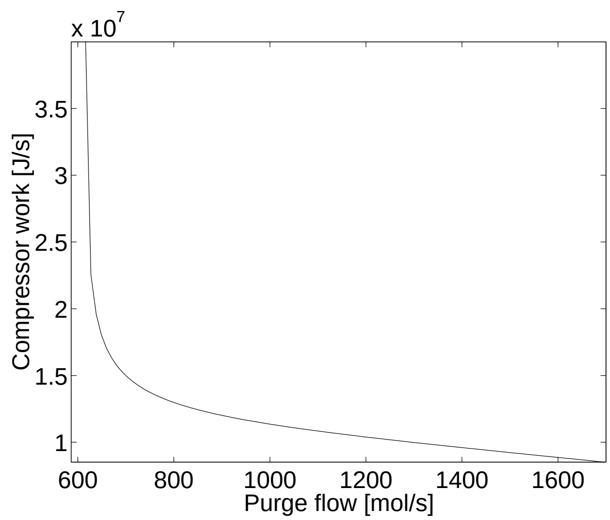
Methanol synthesis loop



One degree of freedom.

The objective contains, production rate, compressor work and purge

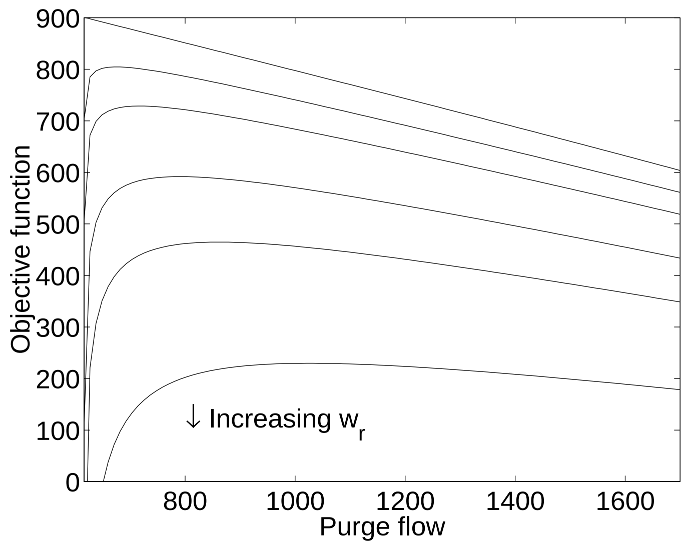




We want production to be as large as possible and use as little compression work as possible:

Simplified objective:

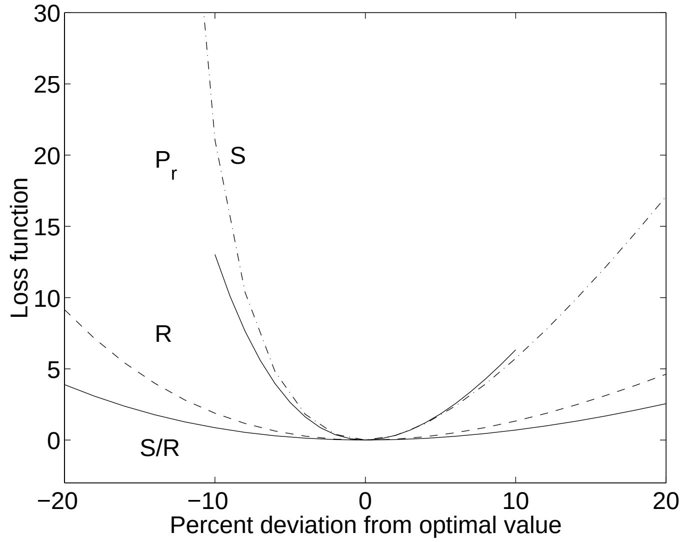
$$J = B - w_r W$$

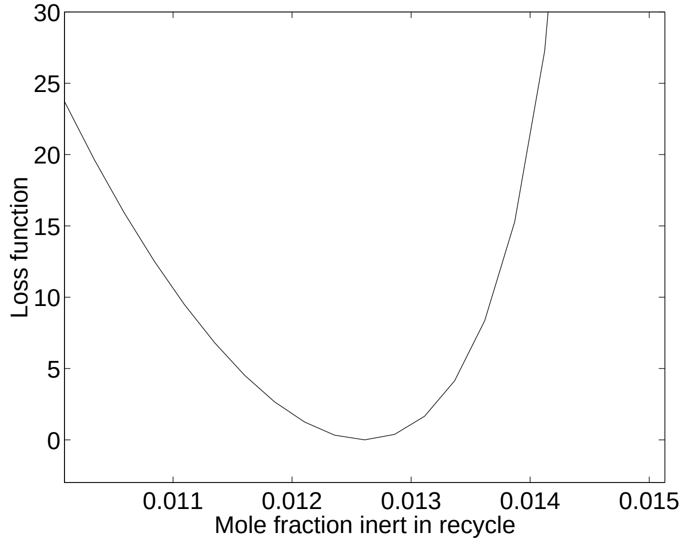


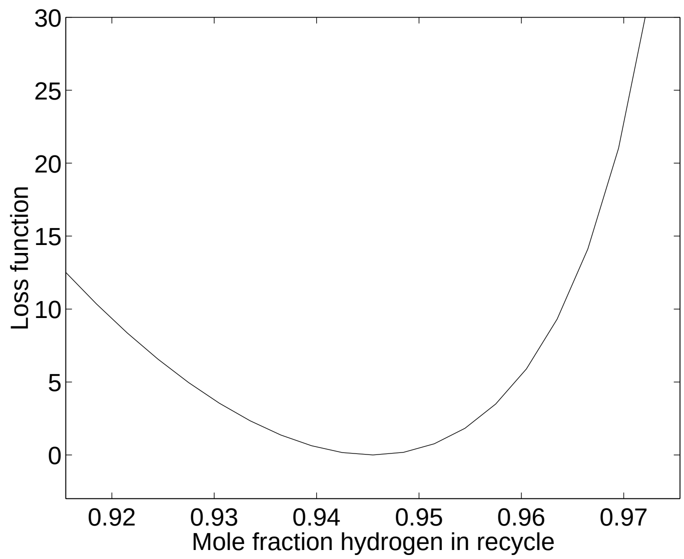
If w_r is small then process optimum will be at a constraint.

Possible candidates for controlled variables are:

- reactor pressure,
- recycle rate,
- purge flow,
- purge flow fraction,
- inert composition,
- hydrogen composition.


Loss function
Percent deviation from optimal value
P r
S
R
S/R


Loss function
Mole fraction inert in recycle


Loss function
Mole fraction hydrogen in recycle

Discussion

- Reactor holdup, will be at constraint if
  - The cost of holdup is small compared to the gain in conversion.

  Floating reactor holdup can have a economic penalty.
- May not be necessary to control "internal compositions" in distillation columns.
- Product compositions should be controlled at their constraints.
- The remaining degree of freedom : Flat objective.
  - Good, selection of controlled variables can be based on other considerations.
  - They could be selected to allow for tighter control of constraints.

  Flat for most,
  - but not for all.
  - large differences between alternatives.
- Do not control inert in purge flow.
- Results carries over to methanol synthesis loop

The concept of self-optimizing control is a useful tool for gaining insight into the process.

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