Economic plantwide control

The critical link in integrated decision making across process operation

Sigurd Skogestad, Vladimiros Minasidis, Julian Straus

Department of Chemical Engineering
Norwegian University of Science and Tecnology (NTNU)
Trondheim, Norway

Rhodes, Greece, 20 June 2016

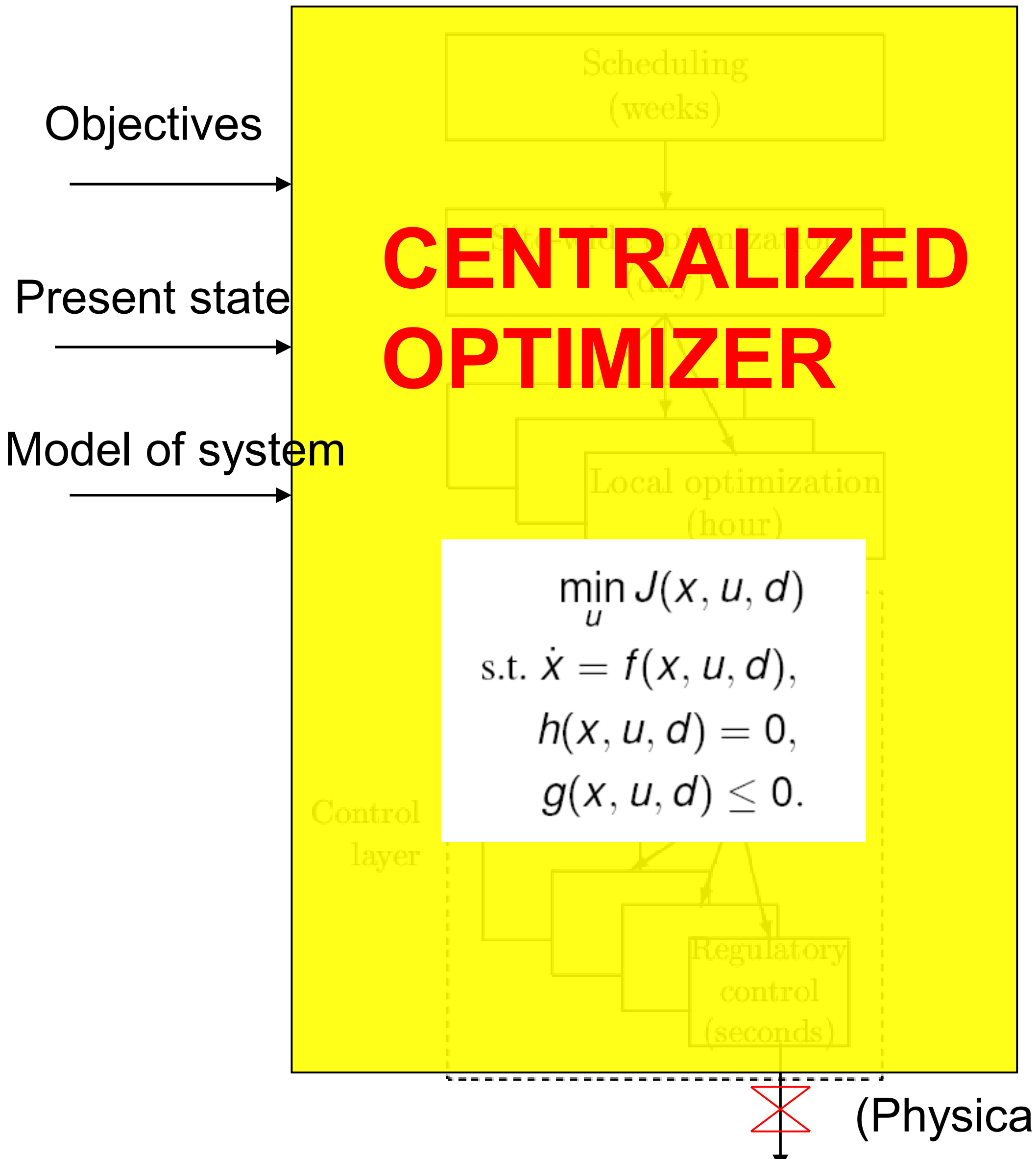
Outline part1

- Objectives of control
- Our paradigm
- Planwide control procedure based on economics
- Active constraints
- Example: Runner
- Selection of primary controlled variables (CV_1=H y)
  - Optimal is gradient, $CV_1=J_u$ with setpoint=0
  - General CV_1=Hy. Nullspace and exact local method
- Throughput manipulator (TPM) location
- Example: Distillation
  - Active constraints regions
- Example: Recycle plants

How we design a control system for a complete chemical plant?

- Where do we start?
- What should we control? and why?
- etc.
- etc.

In theory: Optimal control and operation



$$\min_u J(x,u,d)$$
$$\text{s.t. } \dot{x} = f(x,u,d),$$
$$h(x,u,d) = 0,$$
$$g(x,u,d) \leq 0.$$

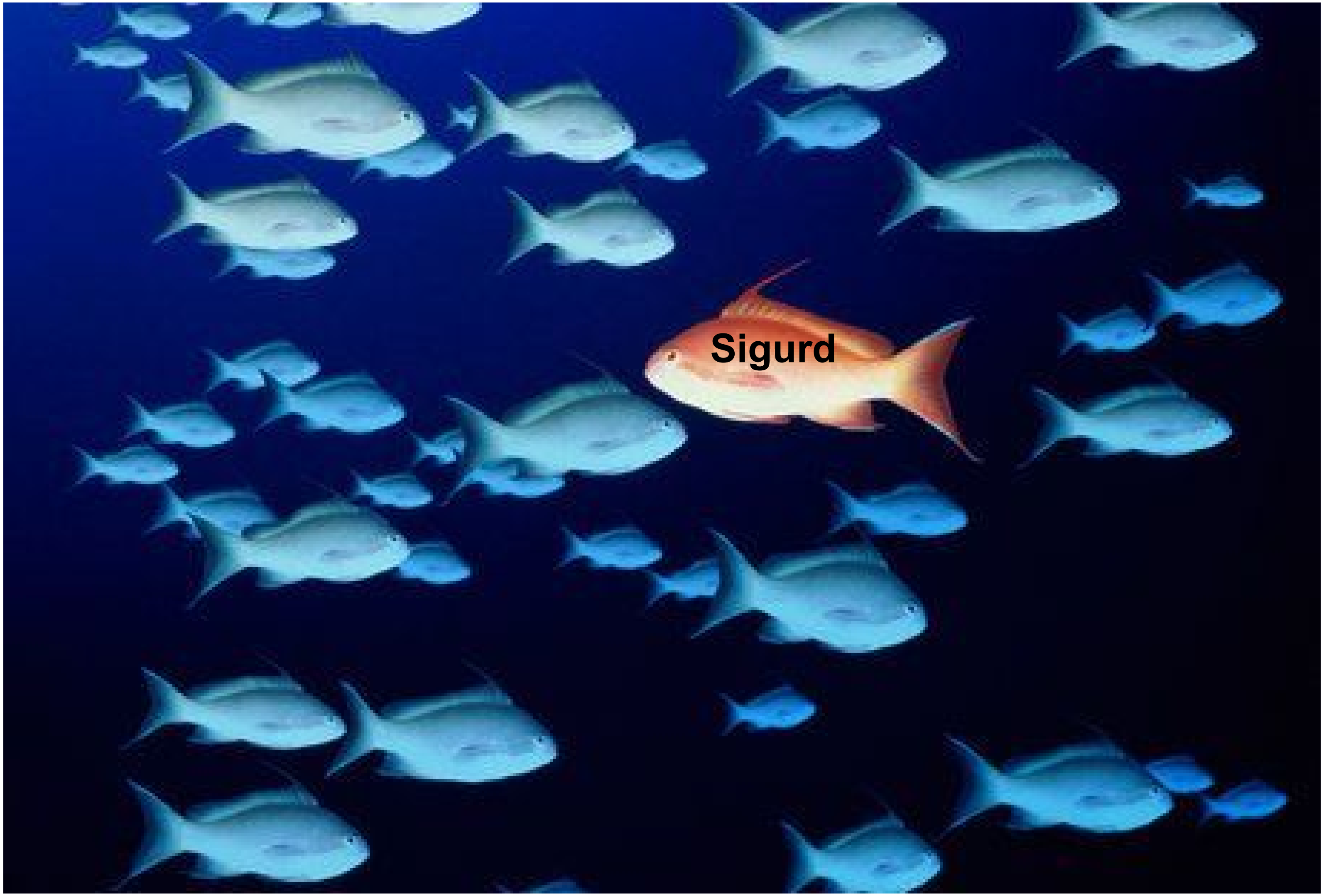
Approach:
- Model of overall system
- Estimate present state
- Optimize all degrees of freedom

Process control:
- Excellent candidate for centralized control

Problems:
- Model not available
- Objectives = ?
- Optimization complex
- Not robust (difficult to handle uncertainty)
- Slow response time

Academic process control community fish pond

Optimal centralized Solution (**EMPC**)



Practice: Engineering systems

- Most (all?) large-scale engineering systems are controlled using hierarchies of quite simple controllers
  - Large-scale chemical plant (refinery)
  - Commercial aircraft
- 100's of loops
- Simple components:

  PI-control + selectors + cascade + nonlinear fixes + some feedforward

Same in biological systems

But: Not well understood

- Alan Foss ("Critique of chemical process control theory", AIChE Journal,1973):

The central issue to be resolved ... is the determination of control system structure. ***Which variables should be measured, which inputs should be manipulated and which links should be made between the two sets?*** *There is more than a suspicion that the work of a genius is needed here, for without it the control configuration problem will likely remain in a primitive, hazily stated and wholly unmanageable form. The gap is present indeed, but contrary to the views of many, it is the theoretician who must close it.*

Previous work on plantwide control:

- Page Buckley (1964) - *Chapter on "Overall process control"* (still industrial practice)
- Greg Shinskey (1967) – *process control systems*
- Alan Foss (1973) - *control system structure*
- Bill Luyben et al. (1975-) – *case studies ; "snowball effect"*
- George Stephanopoulos and Manfred Morari (1980) – *synthesis of control structures for chemical processes*
- Ruel Shinnar (1981-) - *"dominant variables"*
- Jim Downs (1991) - *Tennessee Eastman challenge problem*
- Larsson and Skogestad (2000): *Review of plantwide control*

NTNU

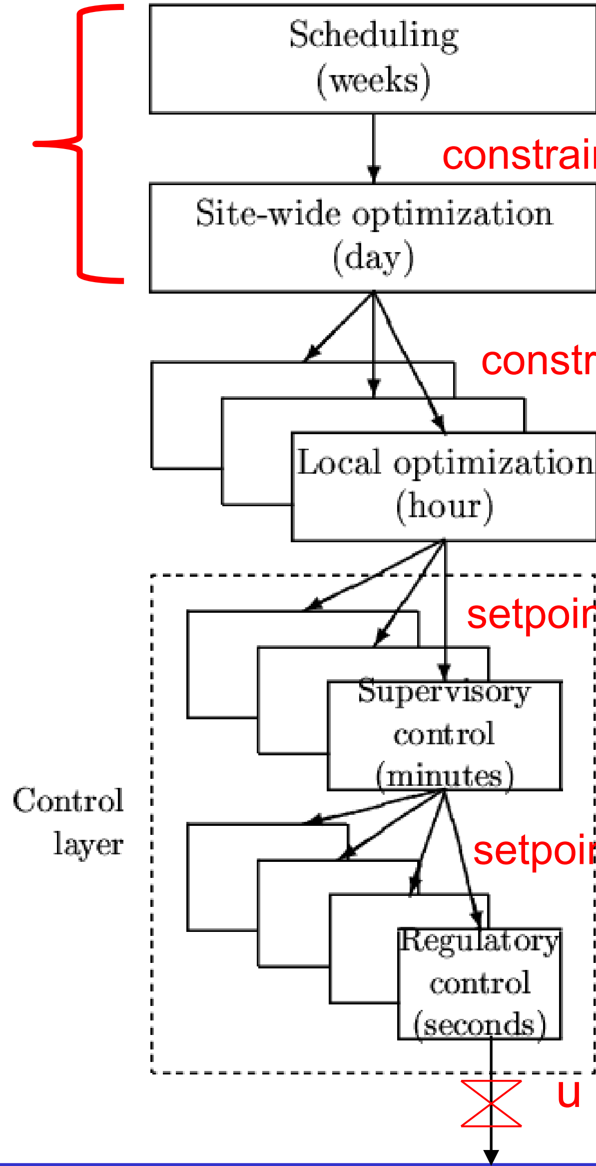
Main objectives control system

1. Economics: Implementation of acceptable (near-optimal) operation
2. Regulation: Stable operation

ARE THESE OBJECTIVES CONFLICTING?

- Usually NOT
  - Different time scales
    - Stabilization fast time scale
  - Stabilization doesn't "use up" any degrees of freedom
    - Reference value (setpoint) available for layer above
    - But it "uses up" part of the time window (frequency range)

Practical operation: Hierarchical structure



Planning

constraints, prices

constraints, prices

setpoints

setpoints

u = valves

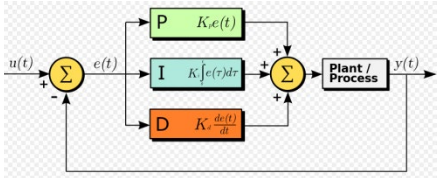
Manager

Process engineer

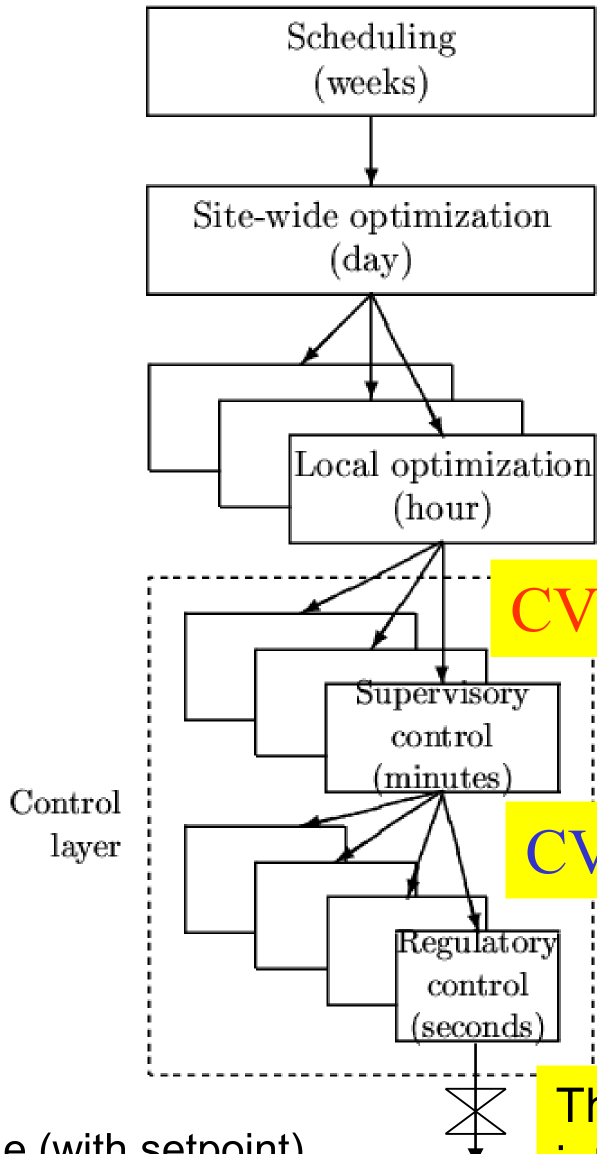
Operator/RTO

Operator/"Advanced control"/MPC

PID-control



Plantwide control: Objectives



OBJECTIVE

RTO — Min J (economics)

CV_{1s}

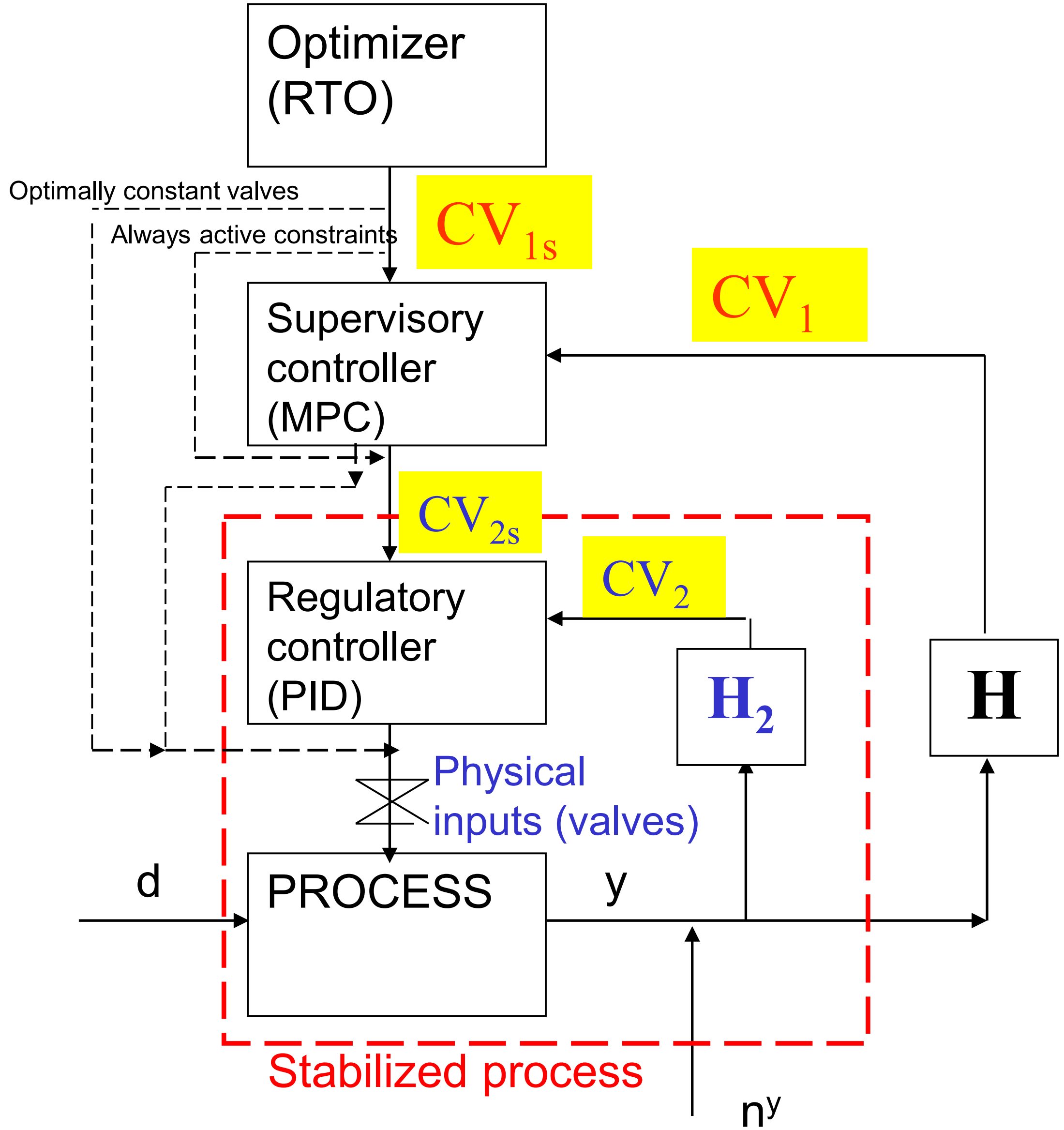
MPC — Follow path (+ look after other variables)

CV_{2s}

PID — Stabilize + avoid drift

The controlled variables (CVs) interconnect the layers

CV = controlled variable (with setpoint)



Degrees of freedom for optimization (usually steady-state DOFs), MVopt = CV1s
Degrees of freedom for supervisory control, MV1=CV2s + unused valves
Physical degrees of freedom for stabilizing control, MV2 = valves (dynamic process inputs)

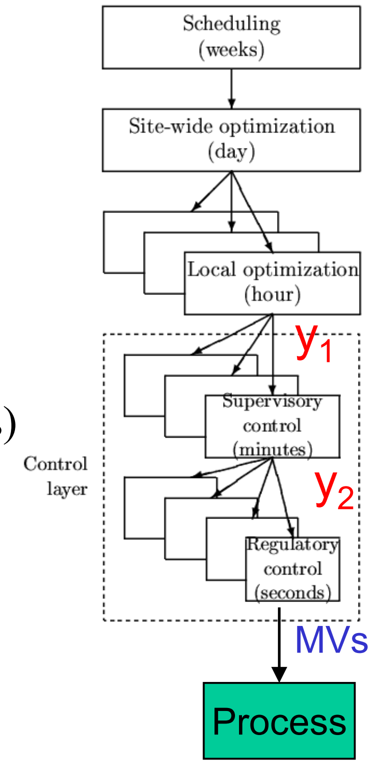
Control structure design procedure

I Top Down (mainly steady-state economics, y_1)

- **Step 1:** Define operational objectives (optimal operation)
  - Cost function J (to be minimized)
  - Operational constraints
- **Step 2:** Identify degrees of freedom (MVs) and optimize for expected disturbances
  - Identify **Active constraints**
- **Step 3**: Select primary "economic" controlled variables $c=y_1$ (CV1s)
  - **Self-optimizing variables (find H)**
- **Step 4:** Where locate the **throughput manipulator (TPM)?**

II Bottom Up (dynamics, y_2)

- **Step 5**: Regulatory / stabilizing control (PID layer)
  - What more to control (y_2; local CV2s)? **Find H_2**
  - Pairing of inputs and outputs
- **Step 6:** Supervisory control (MPC layer)
- **Step 7:** Real-time optimization (Do we need it?)



S. Skogestad, ``Control structure design for complete chemical plants'', *Computers and Chemical Engineering*, **28** (1-2), 219-234 (2004).

Step 1. Define optimal operation (economics)

- What are we going to use our degrees of freedom u (MVs) for?
- Define scalar cost function J(u,x,d)
  - u: degrees of freedom (usually steady-state)
  - d: disturbances
  - x: states (internal variables)

  Typical cost function:

J = cost feed + cost energy – value products

- Optimize operation with respect to u for given d (usually steady-state):

$$\min_u \; J(u,x,d)$$

subject to:

Model equations: $f(u,x,d) = 0$

Operational constraints: $g(u,x,d) < 0$

NTNU

Step S2. Optimize

(a) Identify degrees of freedom

(b) Optimize for expected disturbances

- Need good model, usually steady-state
- Optimization is time consuming! But it is offline
- Main goal: Identify ACTIVE CONSTRAINTS
- A good engineer can often guess the active constraints

Step S3: Implementation of optimal operation

- Have found the optimal way of operation. How should it be implemented?
- **What to control ?** (primary CV's).
  1. Active constraints
  2. Self-optimizing variables (for unconstrained degrees of freedom)

NTNU

Optimal operation of runner

- Cost to be minimized, J=T
- One degree of freedom (u=power)
- What should we control?

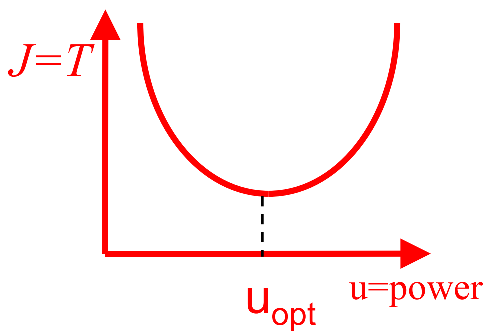
NTNU

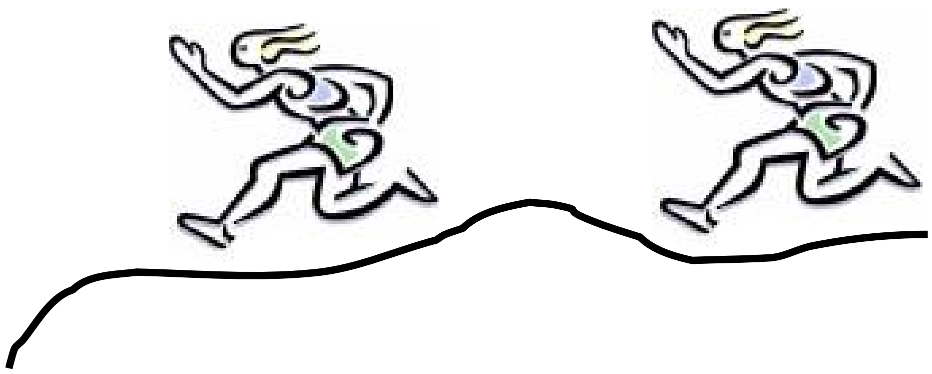
1. Optimal operation of Sprinter

- 100m. J=T
- Active constraint control:
  - Maximum speed (”no thinking required”)
  - CV = power (at max)

2. Optimal operation of Marathon runner

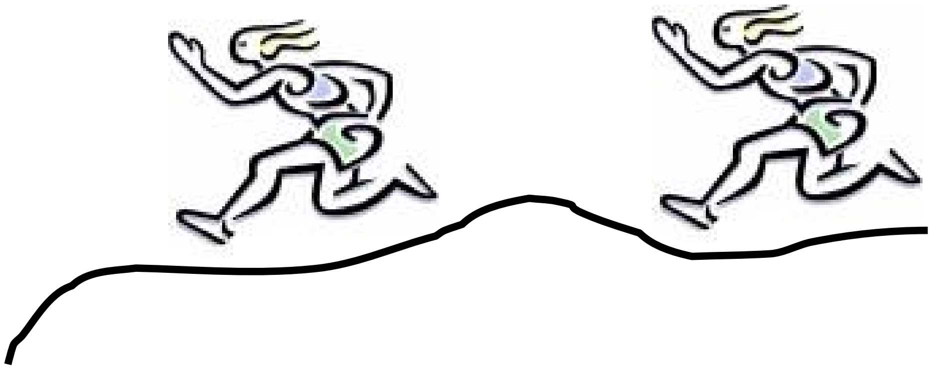
- 40 km. J=T
- What should we control? CV=?
- Unconstrained optimum





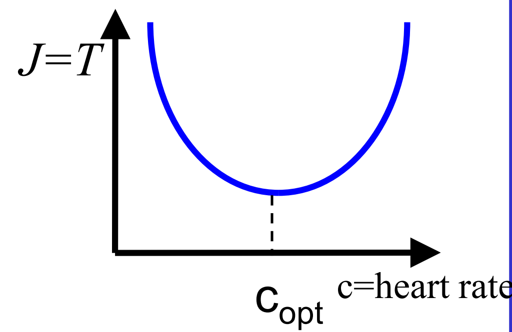
Self-optimizing control: Marathon (40 km)

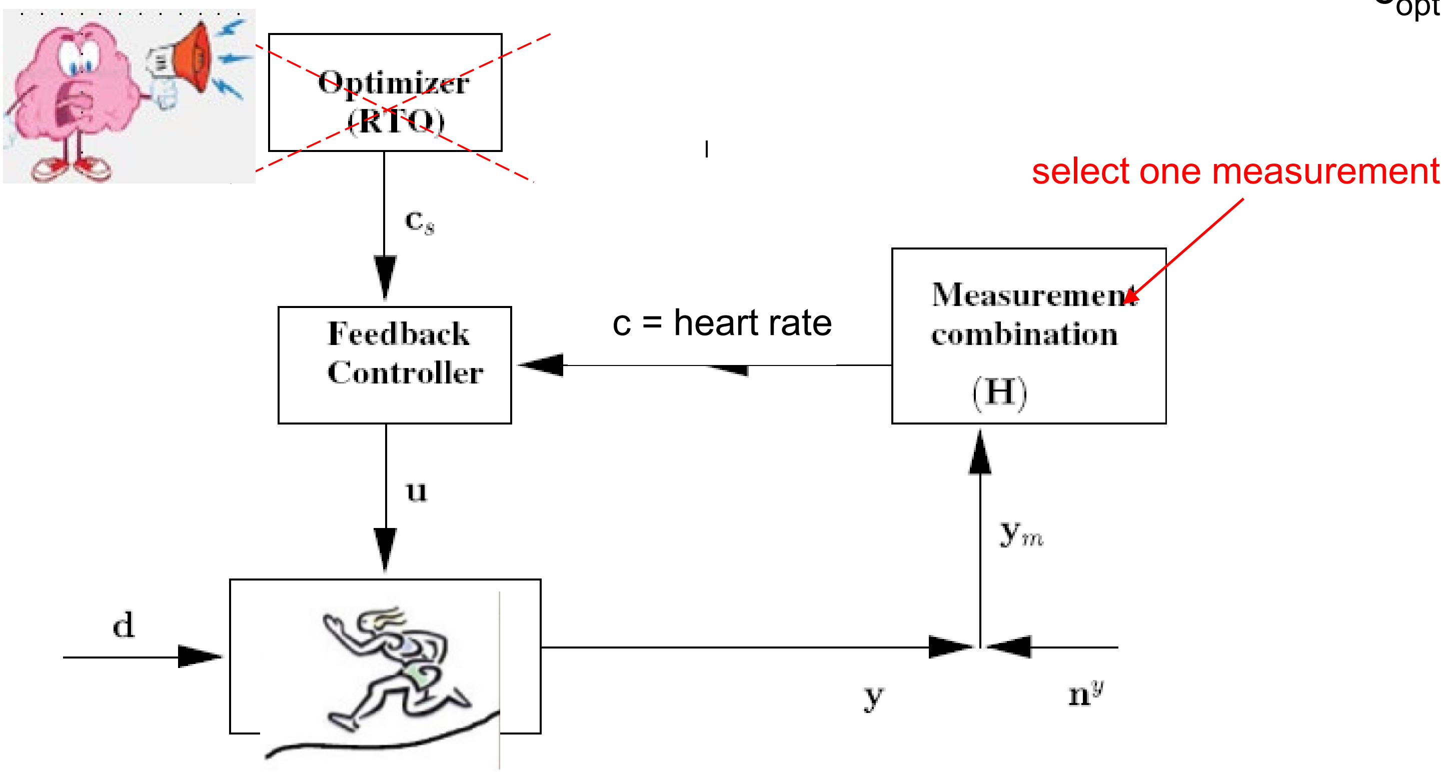
- Any self-optimizing variable (to control at constant setpoint)?
  - c_1 = distance to leader of race
  - c_2 = speed
  - c_3 = heart rate
  - c_4 = level of lactate in muscles



NTNU

Conclusion Marathon runner





- CV = heart rate is good "self-optimizing" variable
- Simple and robust implementation
- Disturbances are indirectly handled by keeping a constant heart rate
- <u>May</u> have infrequent adjustment of setpoint (c_s)

Step 3. What should we control (c)?

Selection of primary controlled variables $y_1=c$

1. **Control active constraints!**
2. **Unconstrained variables: Control self-optimizing variables!**

- Old idea (Morari *et al*., 1980):

"We want to find a function c of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating conditions."

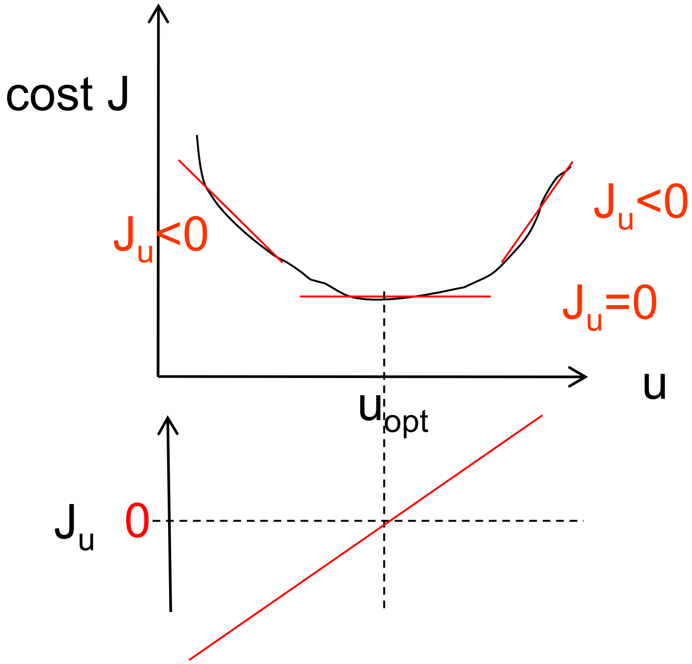
NTNU

NTNU

The ideal “self-optimizing” variable is the gradient, J_u

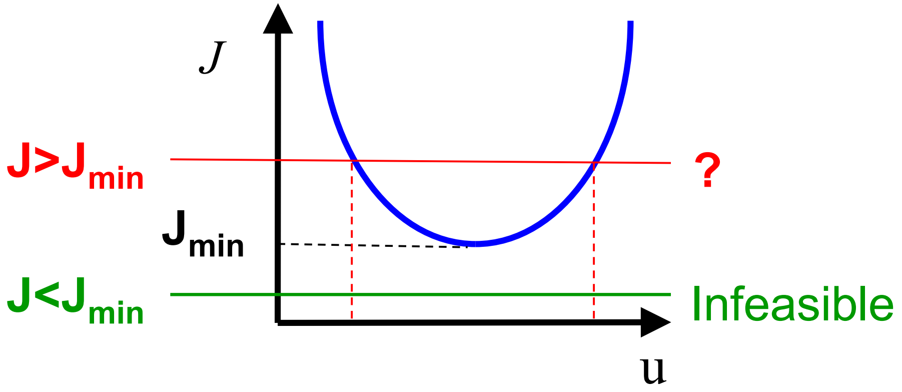
$$c = \partial J/\partial u = J_u$$

- Keep gradient at zero for all disturbances ($c = J_u = 0$)
- Problem: Usually no measurement of gradient



Never try to control the cost function J

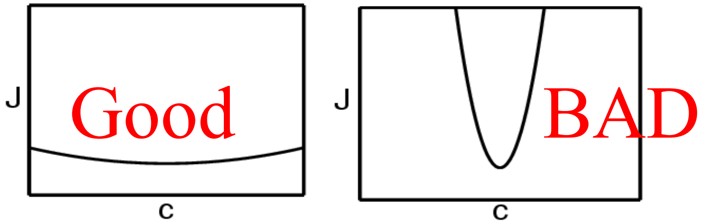
(or any other variable that reaches a maximum or minimum at the optimum)



- Better: control its gradient, Ju, or an associated "self-optimizing" variable.

General: What variable c=Hy should we control? (for self-optimizing control)

1. The *optimal value* of c should be *insensitive* to disturbances
   - Small $F_c = dc_{opt}/dd$
2. c should be easy to measure and control
3. Want "flat" optimum -> The *value* of c should be *sensitive* to changes in the degrees of freedom ("large gain")
   - Large $G = dc/du = HG^y$



(b) Flat optimum: Implementation easy

(c) Sharp optimum: Sensitive to implementation erros

Note: Must also find optimal setpoint for $c=CV_1$

Nullspace method

$$J_u(u,d) = \underbrace{J_u(u_{opt}(d),d)}_{=0} + J_{uu} \cdot (u - u_{opt})$$

$u - u_{opt} = (HG^y)^{-1}(c - c_{opt})$

Here: $c - c_{opt} = \Delta c - \Delta c_{opt}$

where we have introduced deviation variables around a nominal optimal point (c^*, d^*) (where $c^* = c_{opt}(d^*)$)

Assume perfect control of c (no noise): $\Delta c = 0$

Optimal change: $\Delta c_{opt} = H \Delta y_{opt} = HF\Delta d$

Gives: $J_u = -J_{uu}(HG^y)^{-1}HF\Delta d$

$\Rightarrow HF = 0$ gives $J_u = 0$ for any disturbance Δd

- Proof. Appendix B in: Jäschke and Skogestad, "NCO tracking and self-optimizing control in the context of real-time optimization", *Journal of Process Control*, 1407-1416 (2011)

With measurement noise

NTNU

More general ("exact local method")

$$\text{Average loss} = \frac{1}{2}\|M\|_F^2\|$$

$$\text{Worst-case loss} = \frac{1}{2}\bar{\sigma}^2(M)$$

$$M = J_{uu}^{1/2}(HG^y)^{-1}H[FW_d \quad W_{n^y}]\|_2$$

Analytical solution:

$H = G^{yT}(YY^T)^{-1}$ where $Y = [FW_d \quad W_{n^y}]$

- No measurement error: HF=0 (nullspace method)
- With measuremeng error: Minimize GF^c
- Maximum gain rule

Example. Nullspace Method for Marathon runner

u = power, d = slope [degrees]

y_1 = hr [beat/min], y_2 = v [m/s]

$F = dy_{opt}/dd = [0.25 \;\; -0.2]'$

$H = [h_1 \;\; h_2]]$

HF = 0 -> $h_1 f_1 + h_2 f_2 = 0.25\, h_1 - 0.2\, h_2 = 0$

Choose $h_1 = 1$ -> $h_2 = 0.25/0.2 = 1.25$

Conclusion: **c = hr + 1.25 v**

Control **c = constant** -> hr increases when v decreases (OK uphill!)

NTNU

Step 4. Where set production rate?

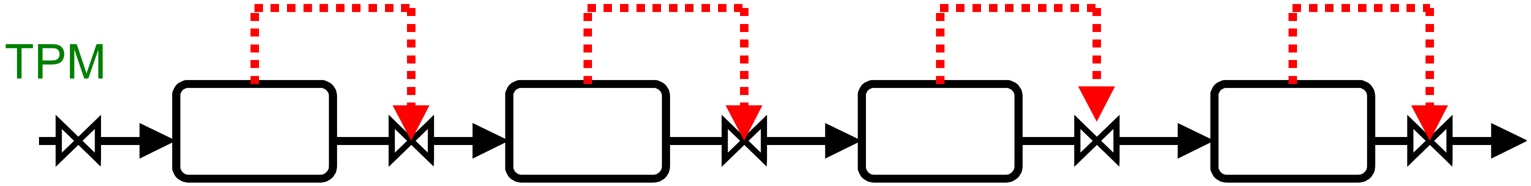
- Where locale the **TPM (throughput manipulator)?**
  - The ”gas pedal” of the process
- Very important!
- Determines structure of remaining inventory (level) control system
- Set production rate at (dynamic) bottleneck
- Link between **Top-down** and **Bottom-up** parts

- NOTE: TPM location is a dynamic issue.

  Link to economics is to improve control of active constraints (reduce backoff)

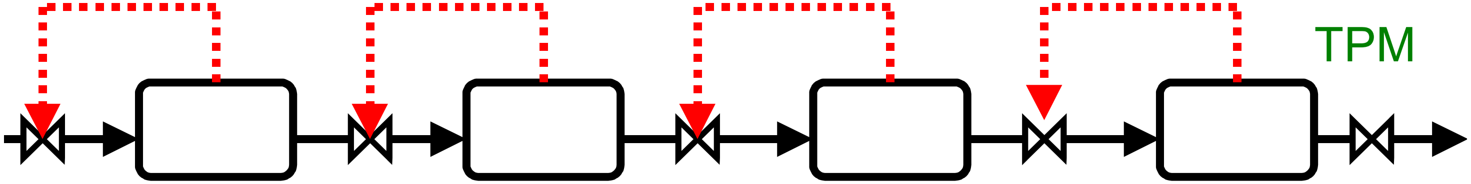
NTNU

Production rate set at inlet : Inventory control in direction of flow*

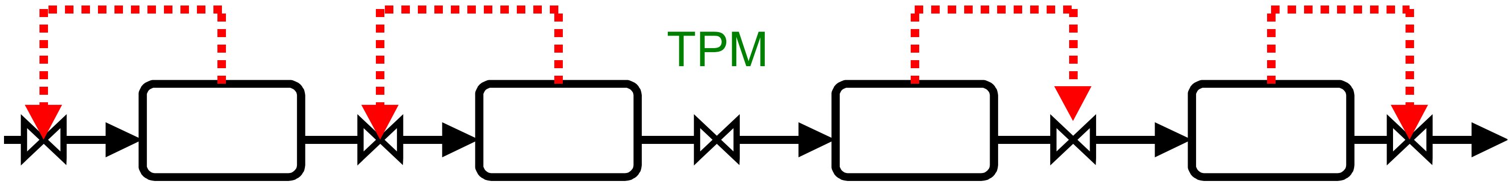


* Required to get “local-consistent” inventory control

Production rate set at outlet: Inventory control opposite flow



Production rate set inside process

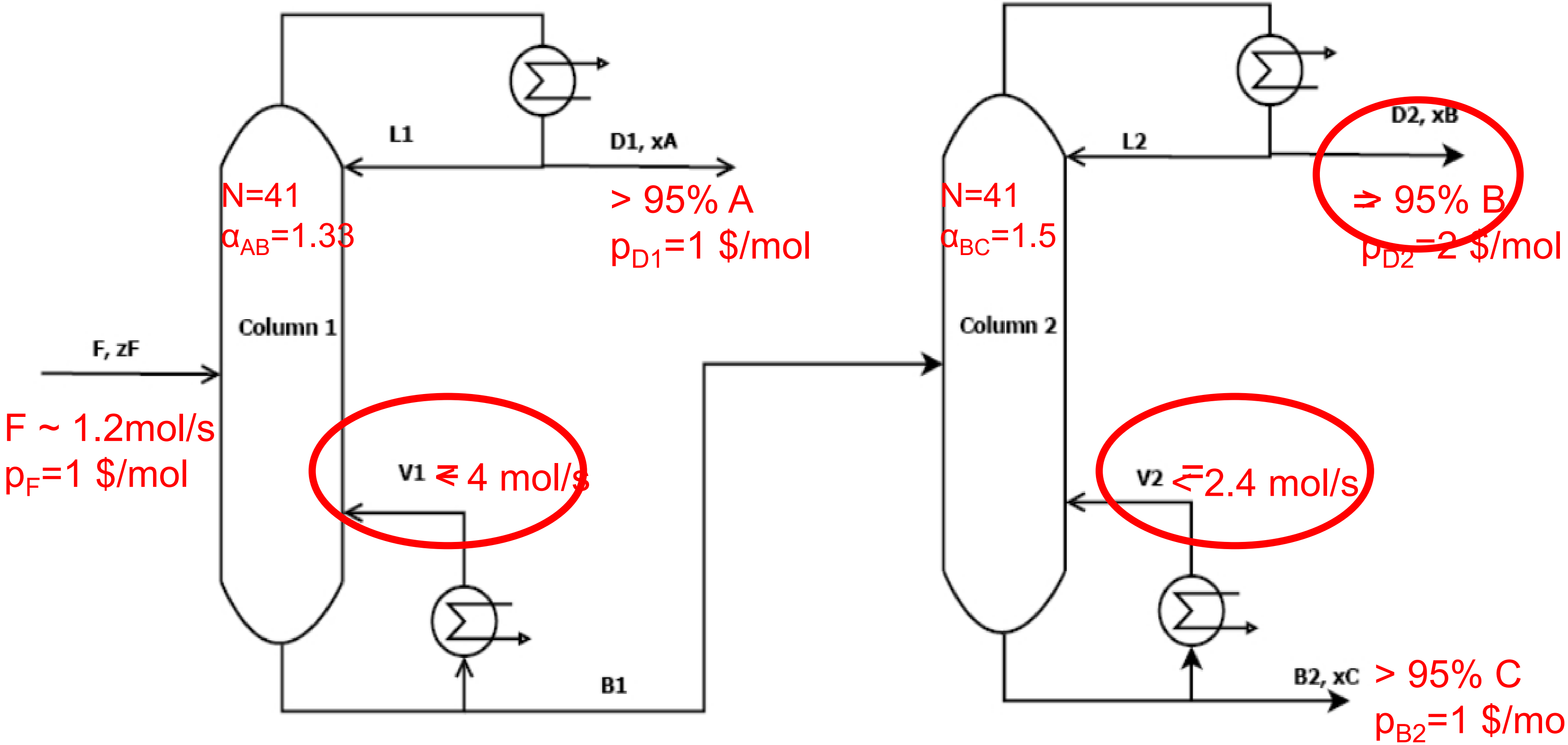


Radiating inventory control around TPM (Georgakis et al.)

Example /QUIZ

Operation of Distillation columns in series

- Cost (J) = - Profit = $p_F F + p_V(V_1+V_2) - p_{D1}D_1 - p_{D2}D_2 - p_{B2}B_2$
- Prices: $p_F=p_{D1}=P_{B2}=1$ \$/mol, $p_{D2}=2$ \$/mol, Energy p_V= 0-0.2 \$/mol (varies)
- With given feed and pressures: 4 steady-state DOFs.
- Here: 5 constraints (3 products > 95% + 2 capacity constraints on V)

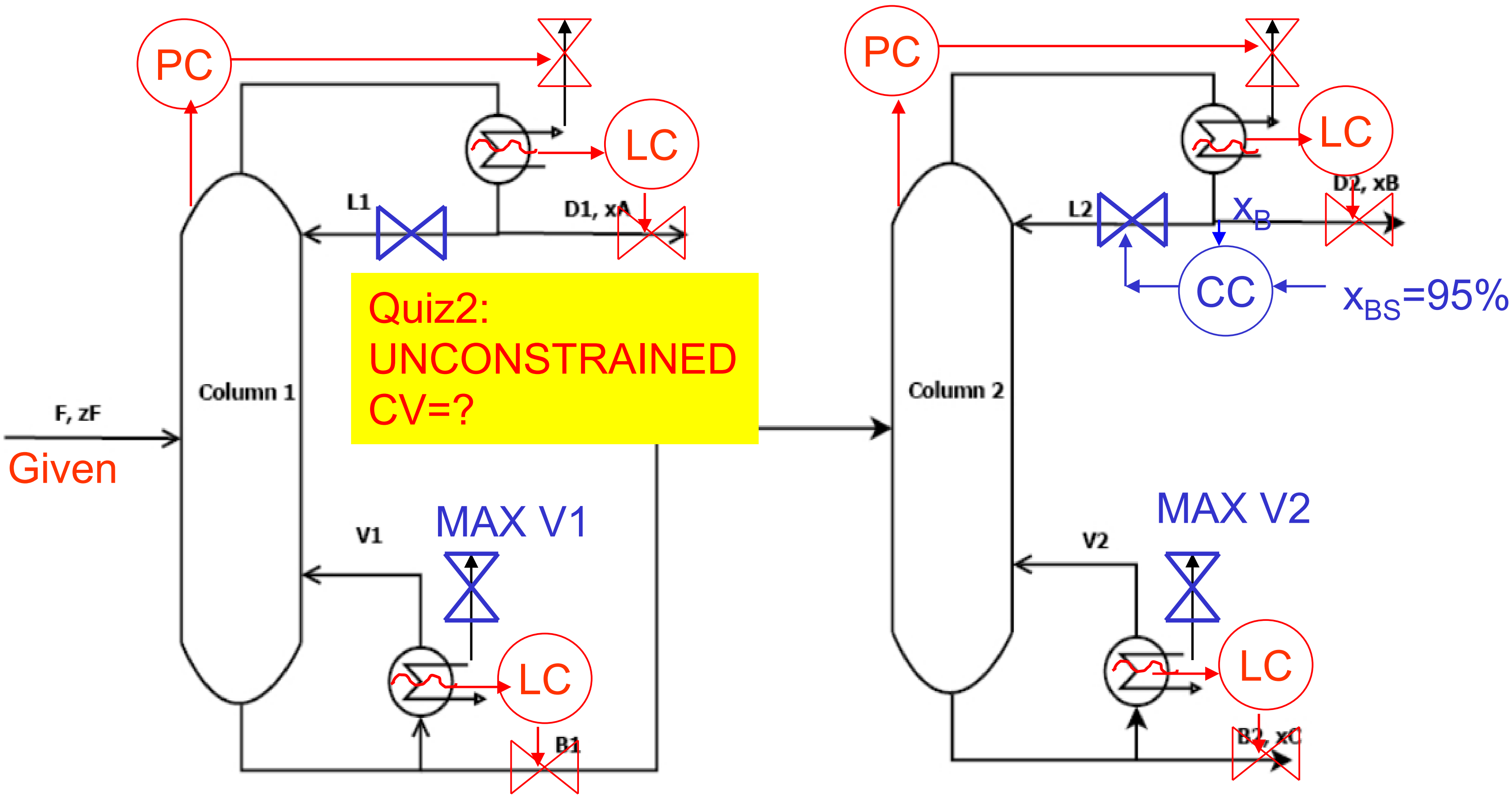


QUIZ: What are the expected active constraints?
1. Always. 2. For low energy prices.

DOF = Degree Of Freedom
Ref.: M.G. Jacobsen and S. Skogestad (2011)

SOLUTION QUIZ1 + new QUIZ2

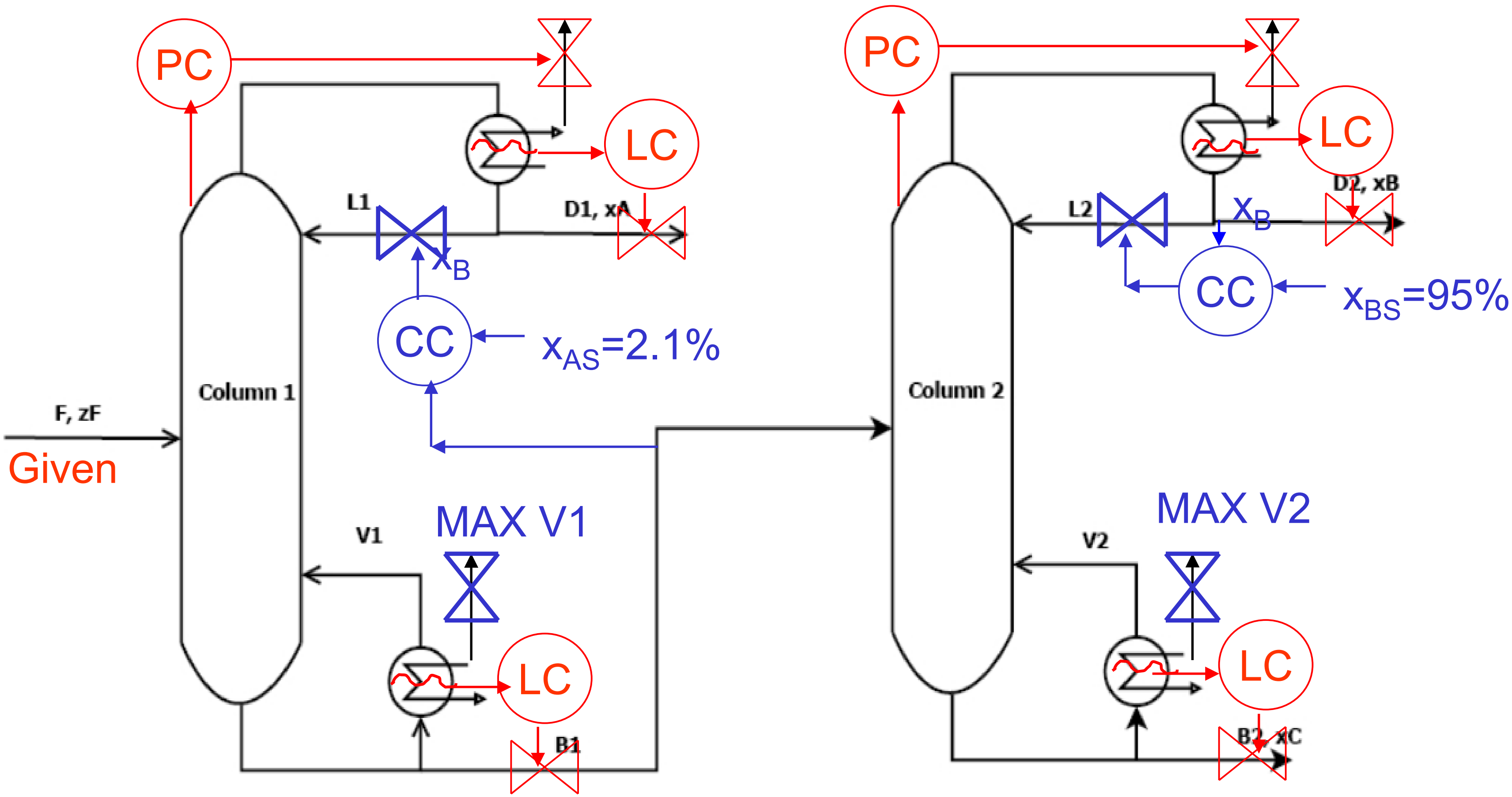
Control of Distillation columns in series



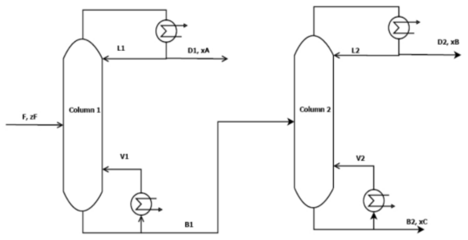
Red: Basic regulatory loops

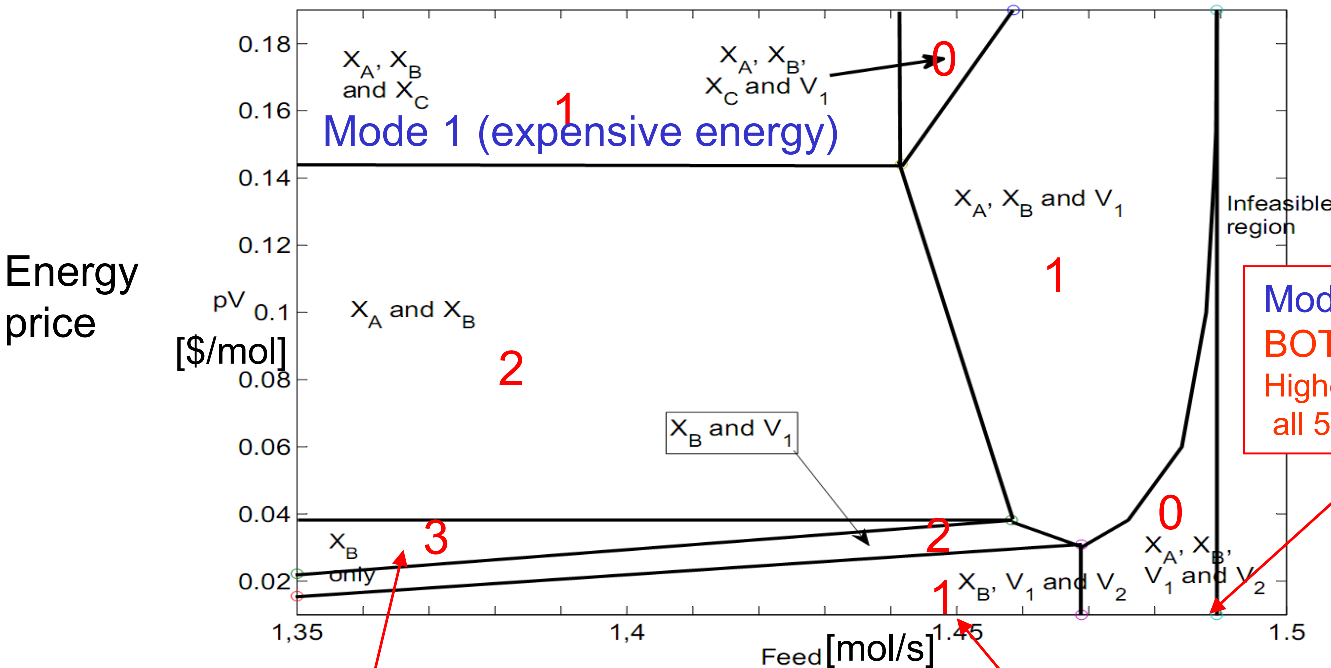
Solution.

Control of Distillation columns. Cheap energy



Active constraint regions for two distillation columns in series





Mode 2: operate at BOTTLENECK. F=1,49
Higher F infeasible because all 5 constraints reached

Mode 1, Cheap energy: 3 active constraints -> 1 remaining unconstrained DOF (L_1) -> Need to find 1 additional CVs ("self-optimizing")

More expensive energy: Only 1 active constraint (xB) ->3 remaining unconstrained DOFs -> Need to find 3 additional CVs ("self-optimizing")

CV = Controlled Variable

How many active constraints regions?

- Maximum: 2^{n_c}

Distillation
n_c = 5
2^5 = 32

n_c = number of constraints

x_B always active
2^4 = 16
-1 = 15

BUT there are usually fewer in practice

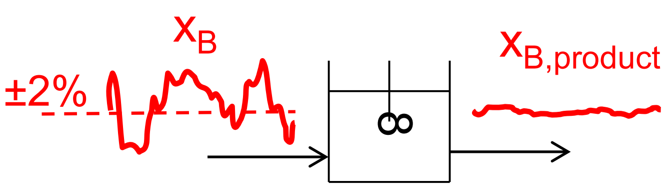
- Certain constraints are always active (reduces effective n_c)
- Only n_u can be active at a given time
  n_u = number of MVs (inputs)
- Certain constraints combinations are not possibe
  - For example, max and min on the same variable (e.g. flow)
- Certain regions are not reached by the assumed disturbance set

In practice = 8

CV = Active constraint

Example back-off.
x_B = purity product > 95% (min.)

- D_1 directly to customer (hard constraint)
  - Measurement error (bias): 1%
  - Control error (variation due to poor control): 2%
  - Backoff = 1% + 2% = 3%
  - Setpoint x_{Bs}= 95 + 3% = 98% (to be safe)
  - Can reduce backoff with better control (“squeeze and shift”)



- D_1 to <u>large</u> mixing tank (soft constraint)
  - Measurement error (bias): 1%
  - Backoff = 1%
  - Setpoint x_{Bs}= 95 + 1% = 96% (to be safe)
  - Do not need to include control error because it averages out in tank

Case study: Recycle plant

CSTR

1^{st} order kinetics

$A \rightarrow B$

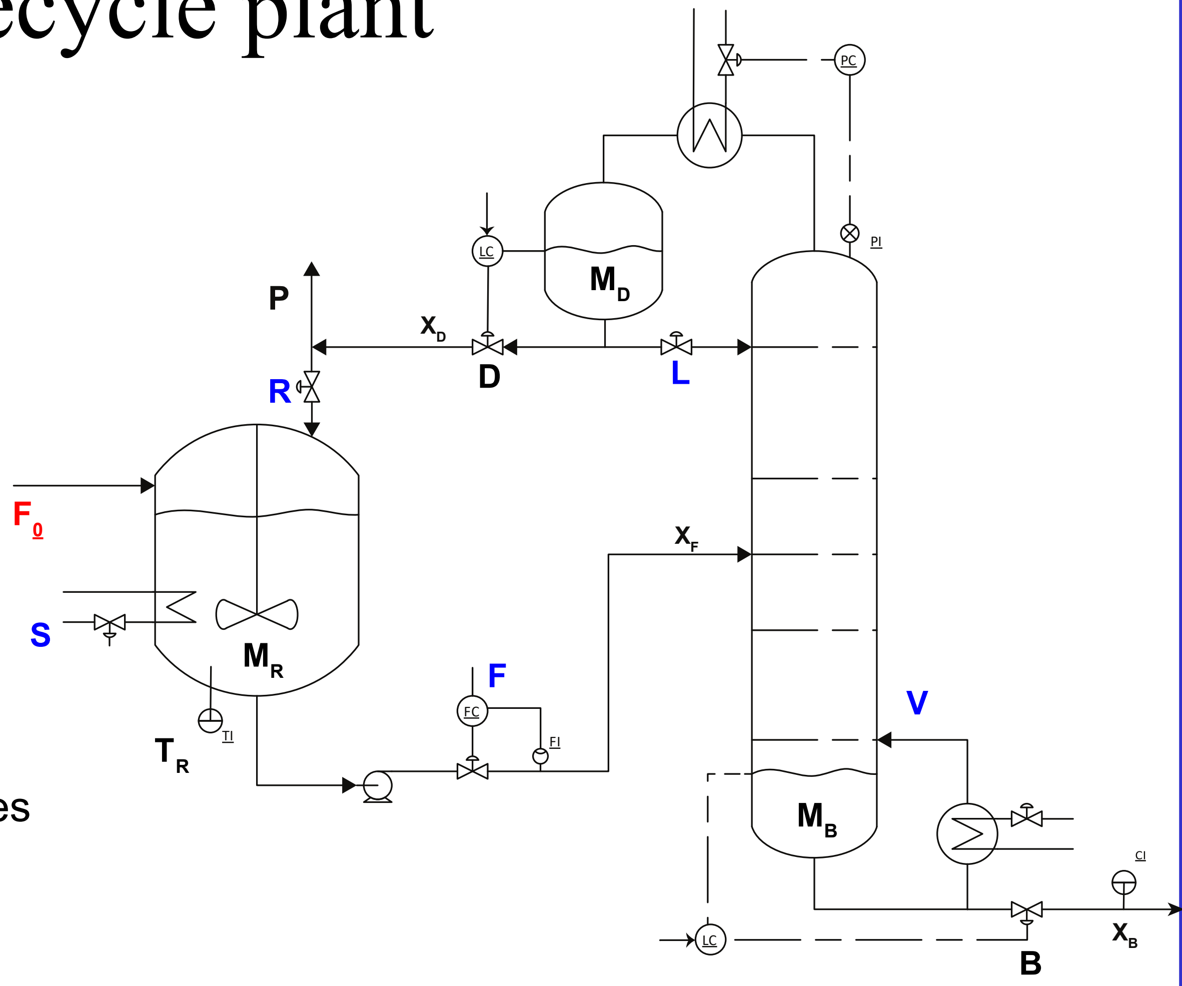
$A \rightarrow 2C$ (undesired)

Column

30 stages
LV - configuration

Assumptions:

- Constant relative volatilities
- Constant molar overflows
- Constant pressure



Based on Luyben.
Details can be found in Jacobsen et. al, [2011]

Step 1: Define operational objectives and degrees of freedom

Cost function:

$$J = p_F F_0 + p_V V - p_P P - p_B B$$

steam cost; cost feed; value products

$$[p_F, p_V, p_P, p_B] = [1, 0.01, 0.5, 2]$$

prices in $/kmol

Operational constraints*:

$x_{B,B} \leq 0.9$ $\quad T_R \leq 390$ K

$M_R \leq 11000$ mol $\quad V \leq 30$ mol/s

$R \geq 0$ mol/s

Degrees of freedom (DOF):

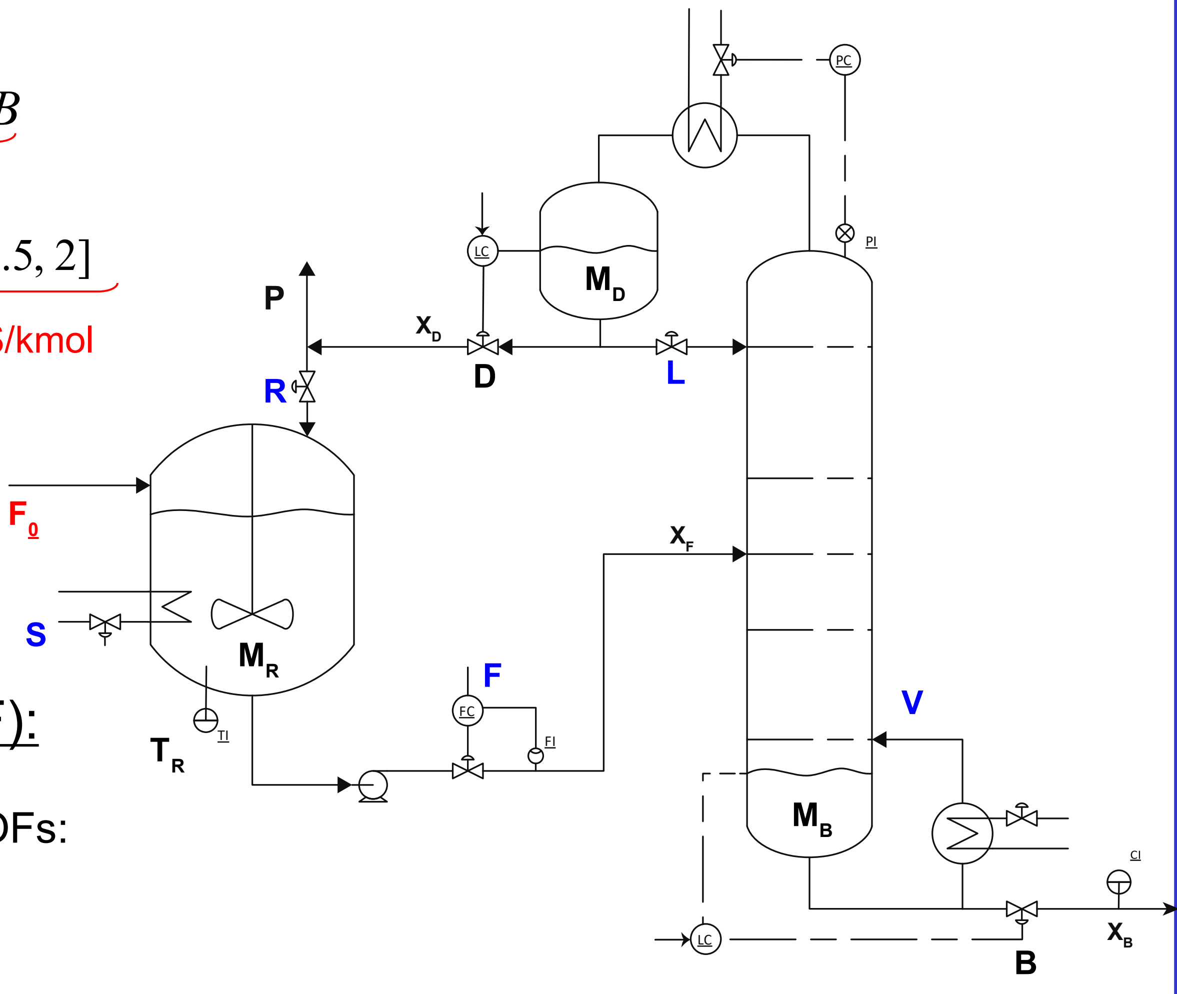
With given F: 4 steady state DOFs:

$$u_{SS} = [L, V, R, S]$$

Disturbances

Main disturbances:

- Feed flow
- Energy price



Step 2: Optimize (by gridding)

Always active:

$$x_{B,B}, T_R, M_R$$

4 active constraints regions (with additional constraints):

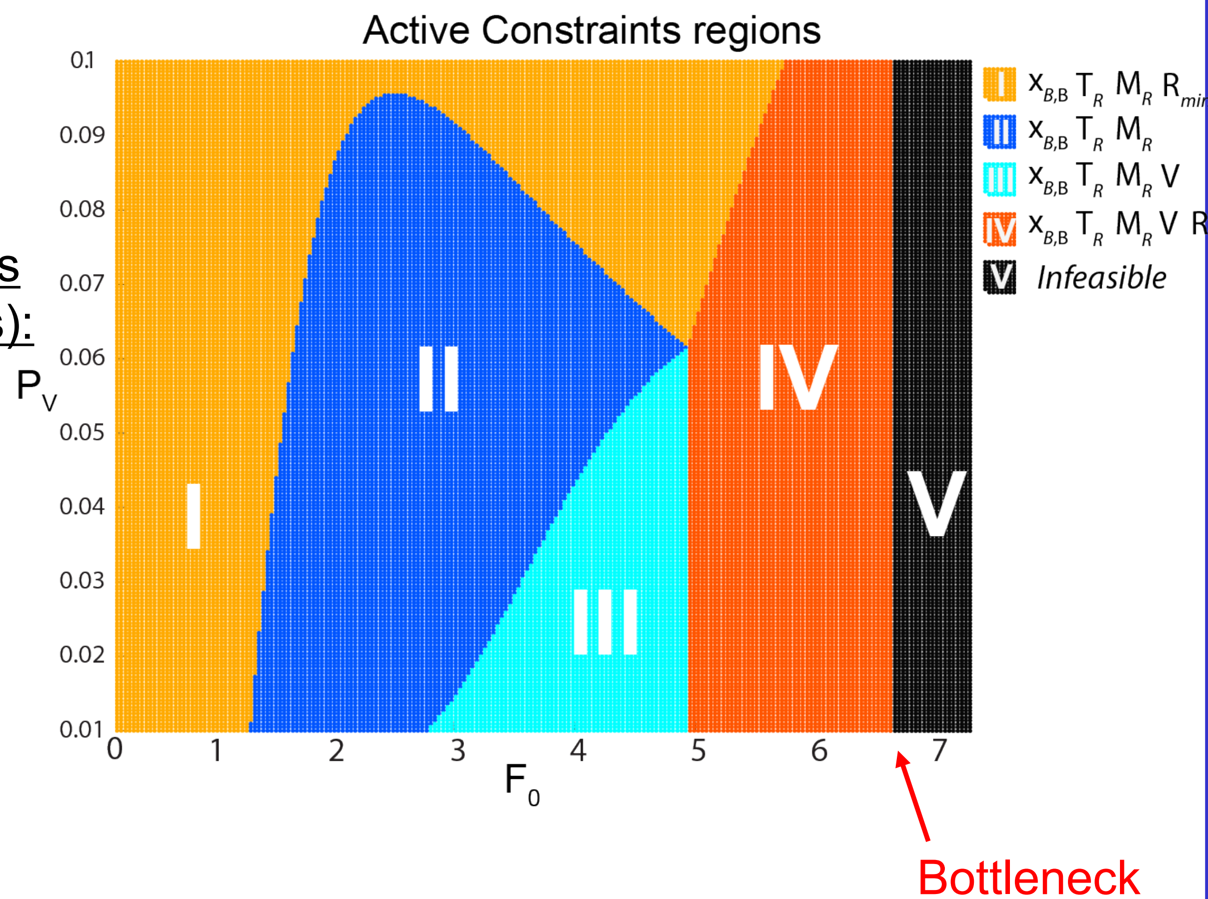
(I) R

(II)

(III) V

(IV) V, R

(V) **Infeasible**



Operational constraints:

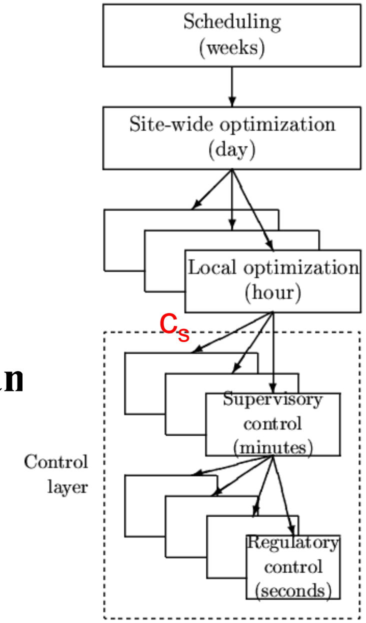
$x_{B,B} \leq 0.9$ $T_R \leq 390$ K

$M_R \leq 11000$ mol $V \leq 30$ mol/s

$R \geq 0$ mol/s

Summary so far:
Systematic procedure for plantwide control

- **Start “top-down” with economics:**
  - Step 1: Define operational objectives and identify degrees of freeedom
  - Step 2: Optimize steady-state operation.
  - Step 3A: Identify active constraints = primary CVs c.
  - Step 3B: Remaining unconstrained DOFs: Self-optimizing CVs c.
  - Step 4: Where to set the throughput (usually: feed)
- **Regulatory control I: Decide on how to move mass through the plan**
  - Step 5A: Propose “local-consistent” inventory (level) control structure.
- **Regulatory control II: “Bottom-up” stabilization of the plant**
  - Step 5B: Control variables to stop “drift” (sensitive temperatures, pressures, ...)
    - Pair variables to avoid interaction and saturation
- **Finally: make link between “top-down” and “bottom up”.**
  - Step 6: “Advanced/supervisory control” system (MPC):
    - CVs: Active constraints and self-optimizing economic variables +
    - look after variables in layer below (e.g., avoid saturation)
    - MVs: Setpoints to regulatory control layer.
    - Coordinates within units and possibly between units



http://www.nt.ntnu.no/users/skoge/plantwide

Summary and references

- The following paper summarizes the procedure:
  - S. Skogestad, ``Control structure design for complete chemical plants'', *Computers and Chemical Engineering*, **28** (1-2), 219-234 (2004).
- There are many approaches to plantwide control as discussed in the following review paper:
  - T. Larsson and S. Skogestad, ``Plantwide control: A review and a new design procedure'' *Modeling, Identification and Control*, **21**, 209-240 (2000).
- The following paper updates the procedure:
  - S. Skogestad, ``Economic plantwide control'', Book chapter in V. Kariwala and V.P. Rangaiah (Eds), *Plant-Wide Control: Recent Developments and Applications",* Wiley (2012).
- Another paper:
  - S. Skogestad "Plantwide control: the search for the self-optimizing control structure'", *J. Proc. Control*, 10, 487-507 (2000).
- More information:

http://www.nt.ntnu.no/users/skoge/plantwide

Part 2. Challenges and open problems (at least to me)

- Oh yes ☺

Challenge: Effective plantwide optimization using detailed models

Status

A. Offline: Optimization to find constraint regions etc. is much more difficult than I expected
   - Hopeless with standard flowsheeting software (Hysys, Aspen, Unisim, etc.)
   - Very difficult also with Matlab, gProms, etc

B. Online: Even more difficult. RTO based on detailed physical has generally failed. Only used on ethylene plants according to Honeywell (Joseph Lu, IFAC WC 2014, Cape Town)

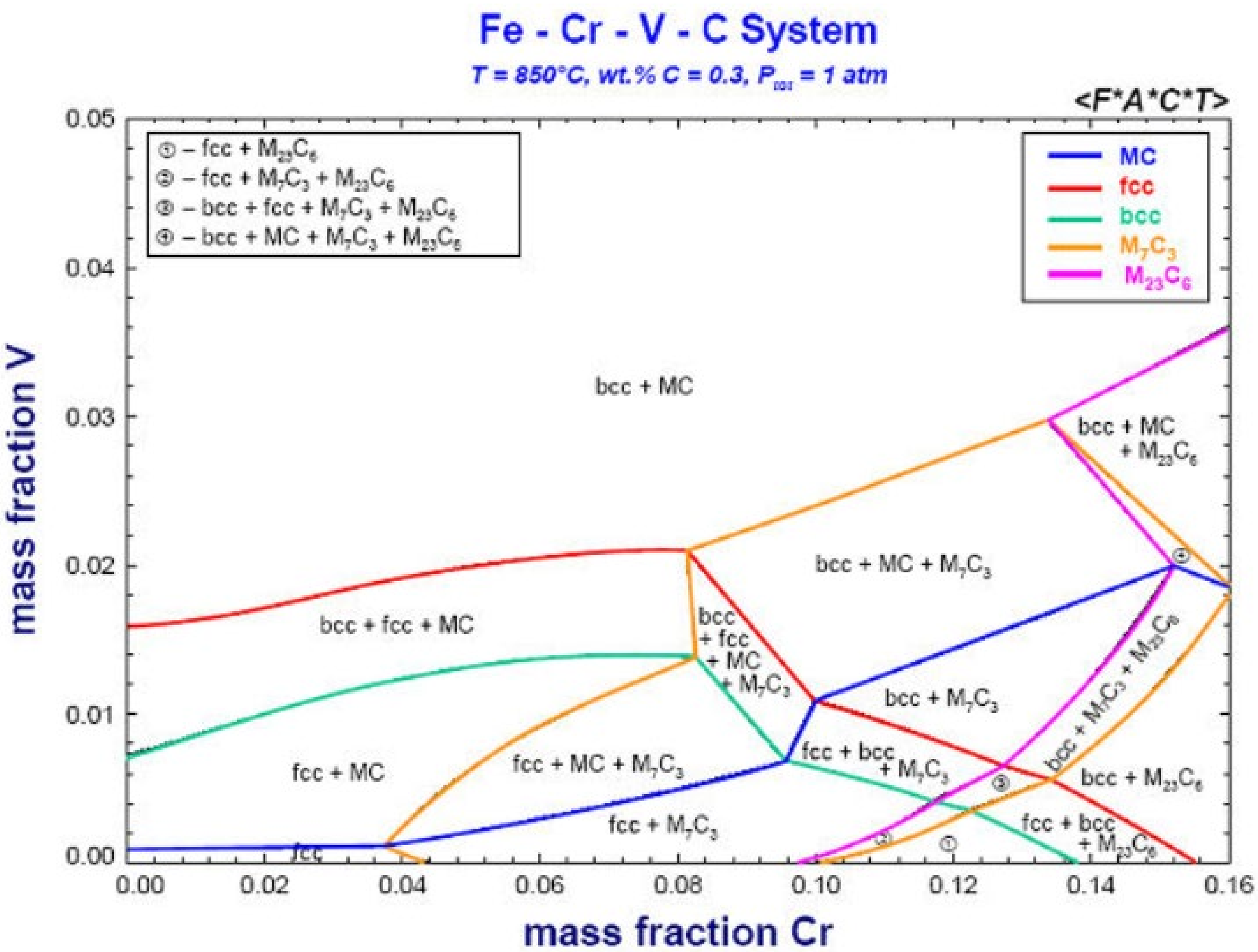
Challenges:

1. Effective off-line optimization and generation of **active constraints regions**
2. Models that are suited for optimization
   - **«Surrogate» models**

RTO = Real-time optimization (steady state)

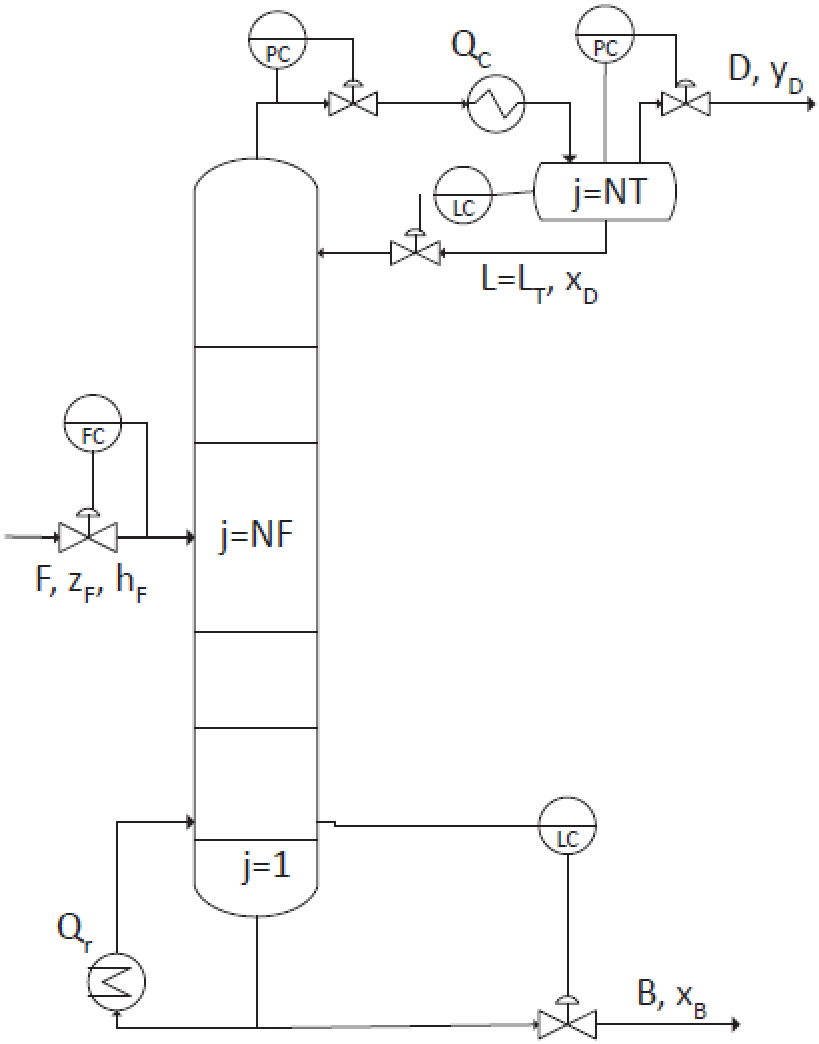
Challenge 1: Find active constraint regions

Phase diagram = Active contraint region map

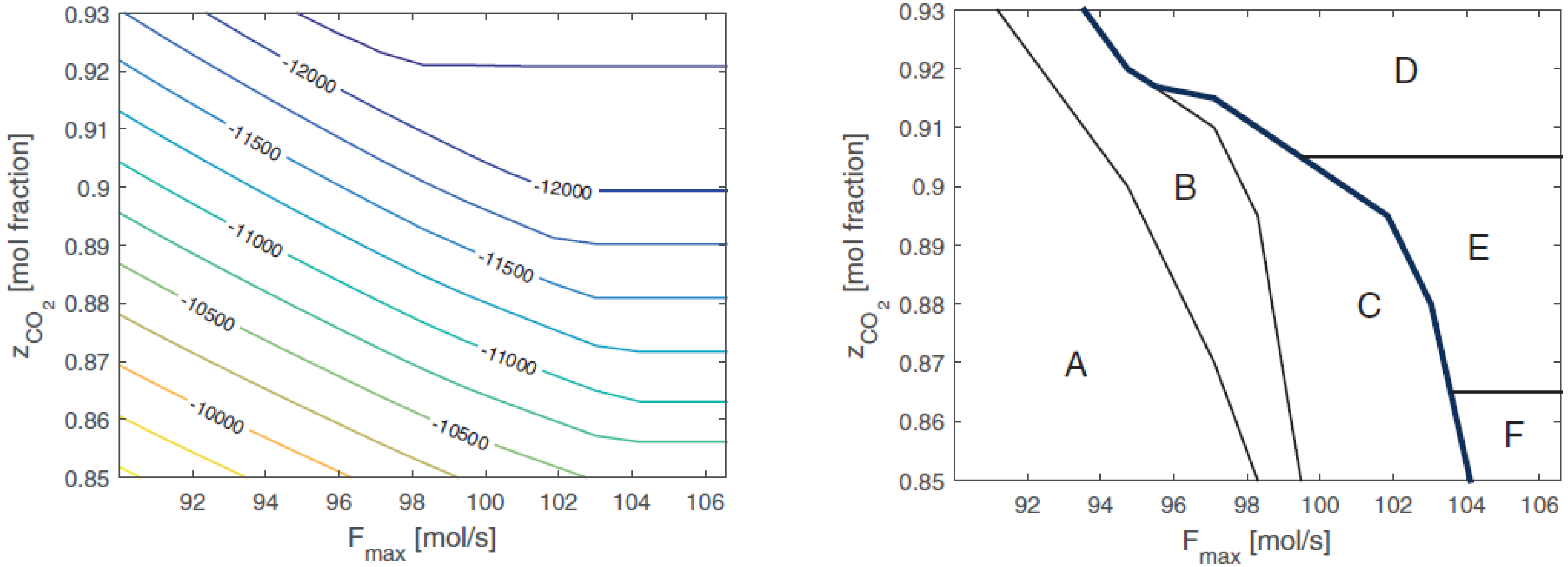


Same topology as for «our» active constraint regions
Phase «active»: Corresponding phase equilibrium equations are active, f=0

CO2-stripper case study



Matlab model



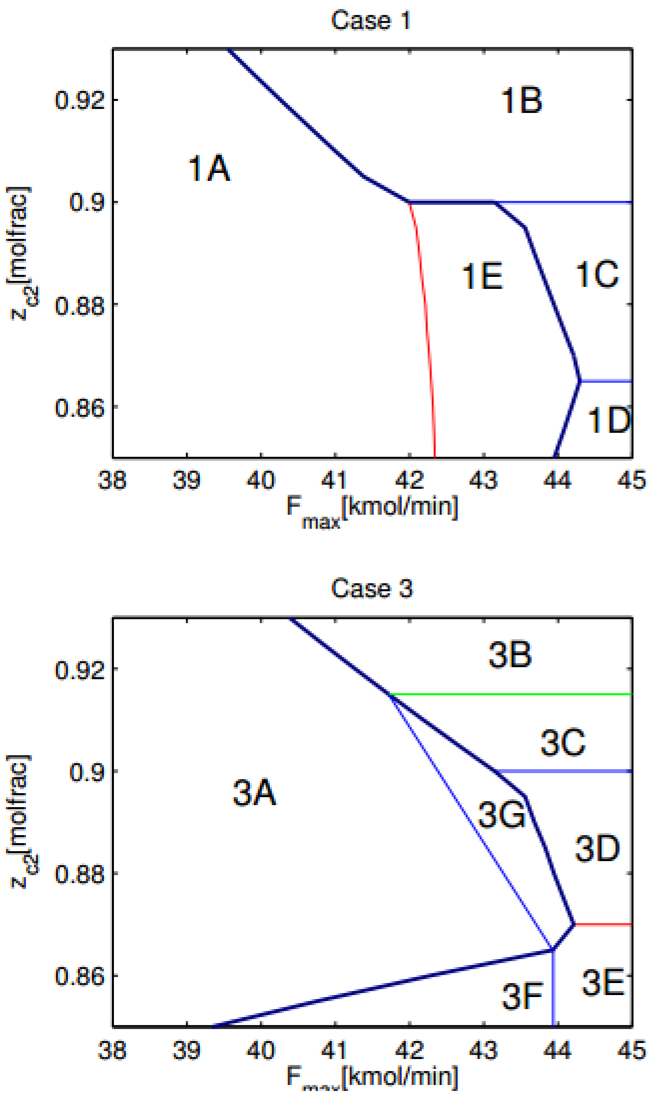
(a) Effect of disturbances on cost function [$ /h].

(b) Active constraints regions

Figure 3: Optimization results for CO_2-stripper.

Table 1: Active constraints regions for CO_2-stripper

Region	Active Constraints
A	WI_{min}, F_{max}
B	WI_{min}, F_{max}, $x_{B,max}$
C	$x_{B,max}$, F_{max}, $Q_{r,max}$
D	WI_{max}, B_{max}
E	$x_{B,max}$, WI_{max}, $Q_{r,max}$
F	$x_{B,max}$, SP_{max}, $Q_{r,max}$



ble 4.3: Active constraints for regions in fig

Region	Active constrains
1A	xB_{max}, WI_{min}, F_{max}
1B	xB_{max}, WI_{min}, B_{max}
1C	xB_{max}, WI_{max},Q_{Rmax}
1D	xB_{max}, SP_{max},Q_{Rmax}
1E	xB_{max}, Q_{Rmax},F_{max}
2A	xB_{max}, WI_{min},F_{max}
2B	B_{max},F_{max}
2C	B_{max}, WI_{max}
2D	xB_{max},WI_{max}, Q_{Rmax},
2E	xB_{max}, Q_{Rmax},SP_{max}
2F	xB_{max}, Q_{Rmax}, F_{max}
3A	WI_{max}, F_{max}
3B	WI_{max}, B_{max}
3C	WI_{max}, B_{max}, Q_{Rmax}
3D	WI_{max}, xB_{max}, Q_{Rmax}
3E	WI_{max}, xB_{max},SP_{max}
3F	WI_{max}, SP_{max}
3G	WI_{max}, Q_{Rmax}

NTNU

2. Surrogate steady-state models for efficient and accurate flowsheet optimization

– hysys/Aspen + standard optimization (build-in, Matlab/fmincon, Excel) is not working

2. Surrogate steady-state models for efficient and accurate flowsheet optimization

- Unit by unit
- Connections are linear, Out1 = In 2
- Main problem: Dimension too high
  - Independent variables: F_i + p,T for each feed stream + u's (e.g. Q) + d's
  - Dependent variables: F_i + p,T for each product stream
  - But: Need max. 4-6 independent variables for most surrogate models (table look-up, splines), (maybe may allow more for polynmials and neural nets ?? But I doubt it)
- Suggested approach
  - First introduce material balances (linear) with extent of reaction as independent variable
  - Use PLS to find additional linear relationships
  - Remaining (including extent of reaction) nonlinear surrogate models
- Must also reduce required range of variables (for gridding)
  - No need to generate data/samples in regions where the system will never operate.
  - To avoid this: Introduce change in independent variables, e.g. Q->T
  - Can base this in existing control structure (or more generally: self-optimizing control ideas)

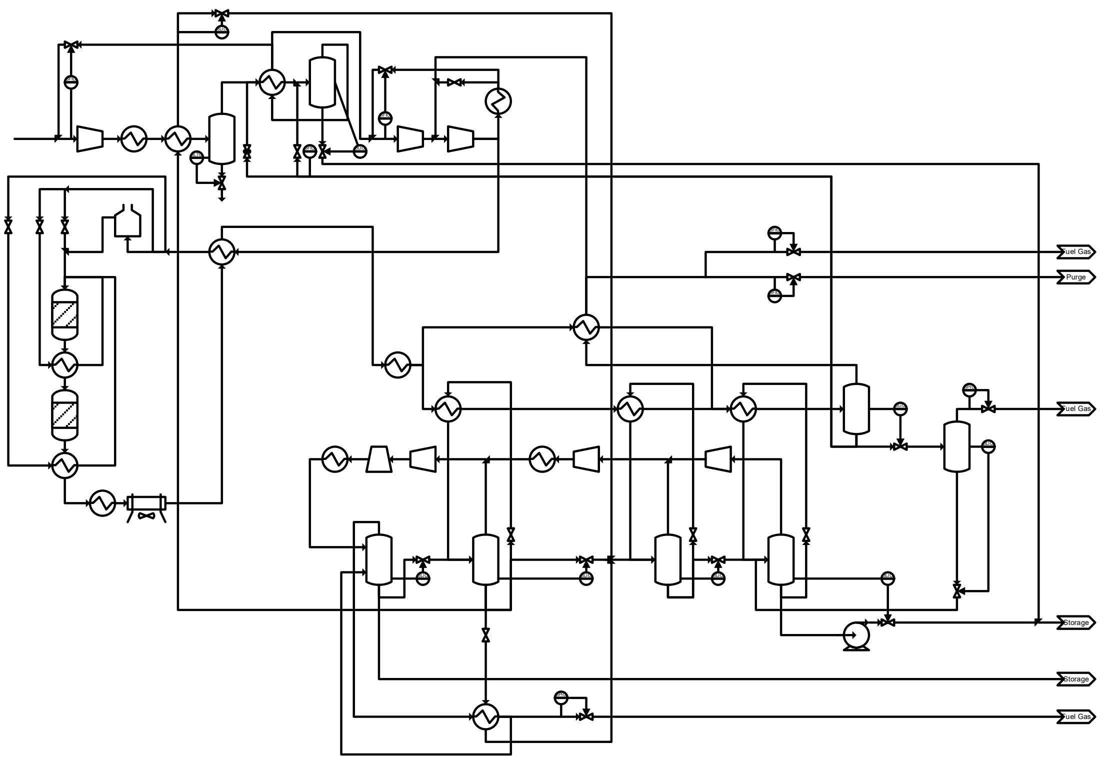
NTNU

Alternative approaches

- Additional sampling during optimization
- ..
- ..
- ..

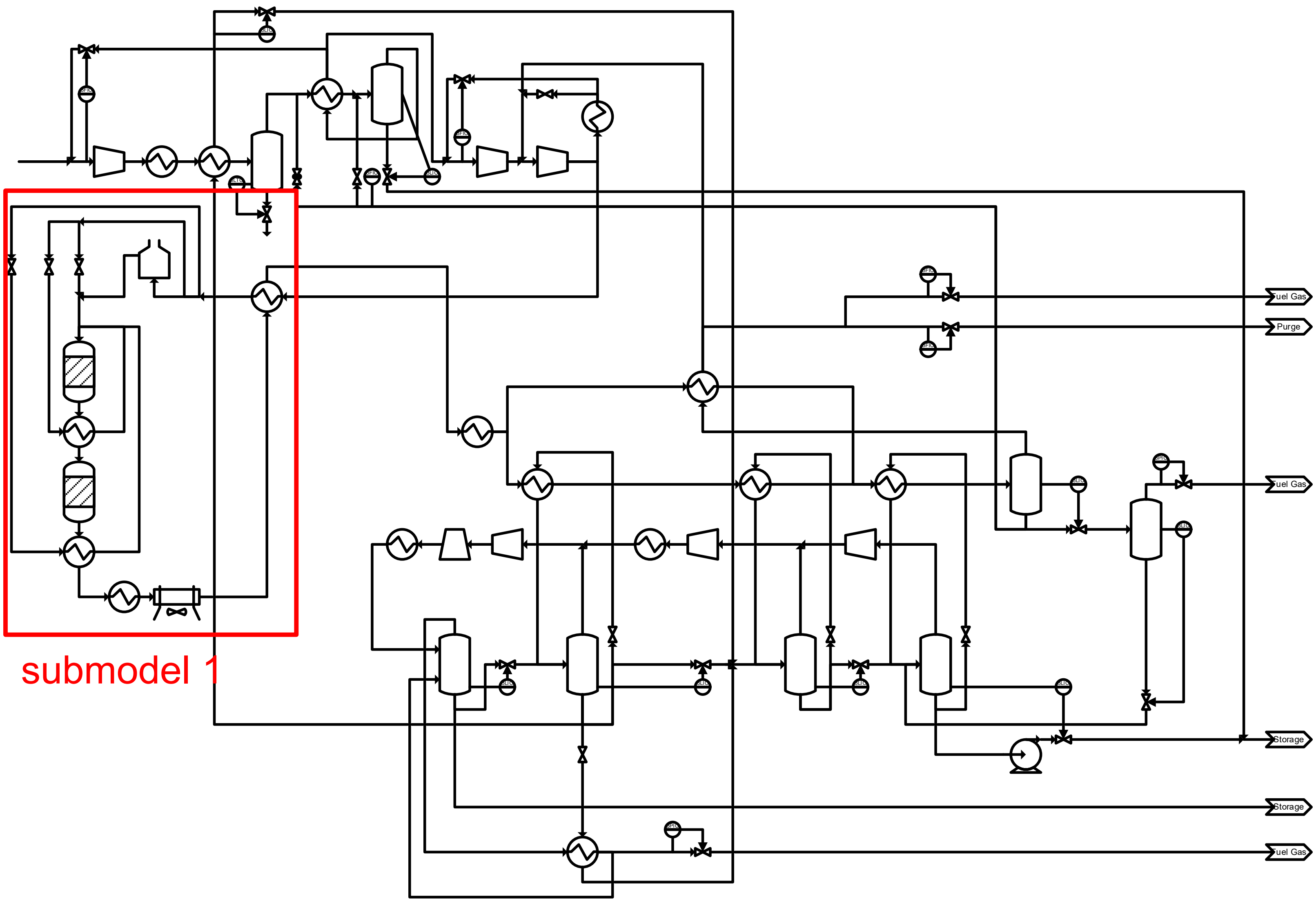
Ammonia synthesis optimization

- Works reasonable with simplified Matlab model
- Hopeless with Hysys model

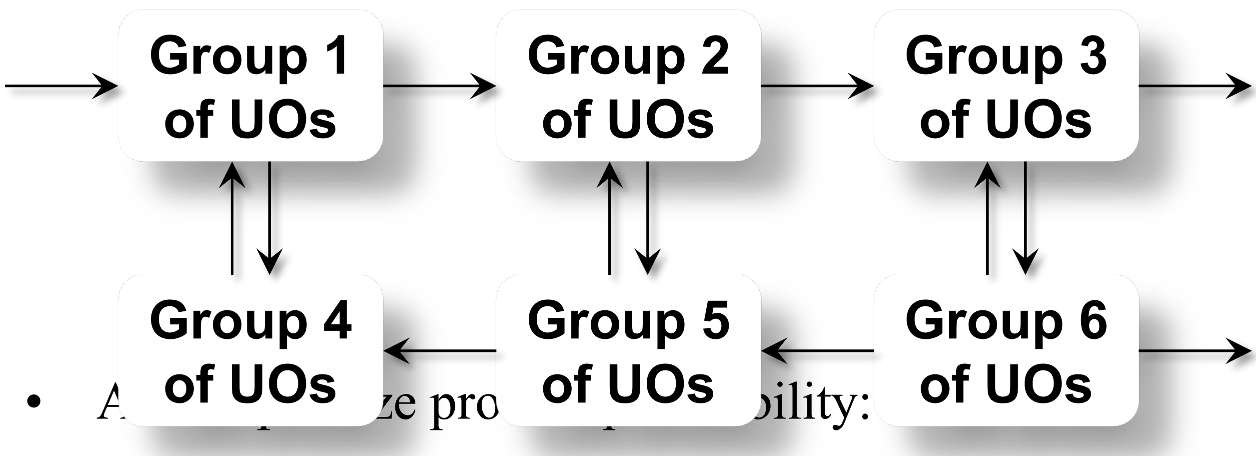


Note: Ammonia reactor section only

Ammonia plant optimization



- Integrated flowsheet in commercial Flowsheeting software



- A ... ze pro ... bility:

$$\min_u J(x,u,d)$$
$$\text{s.t. } f(x,u,d) = 0 \qquad (1)$$
$$g(x,u,d) \le 0$$

NTNU

Separation of flowsheets into submodels

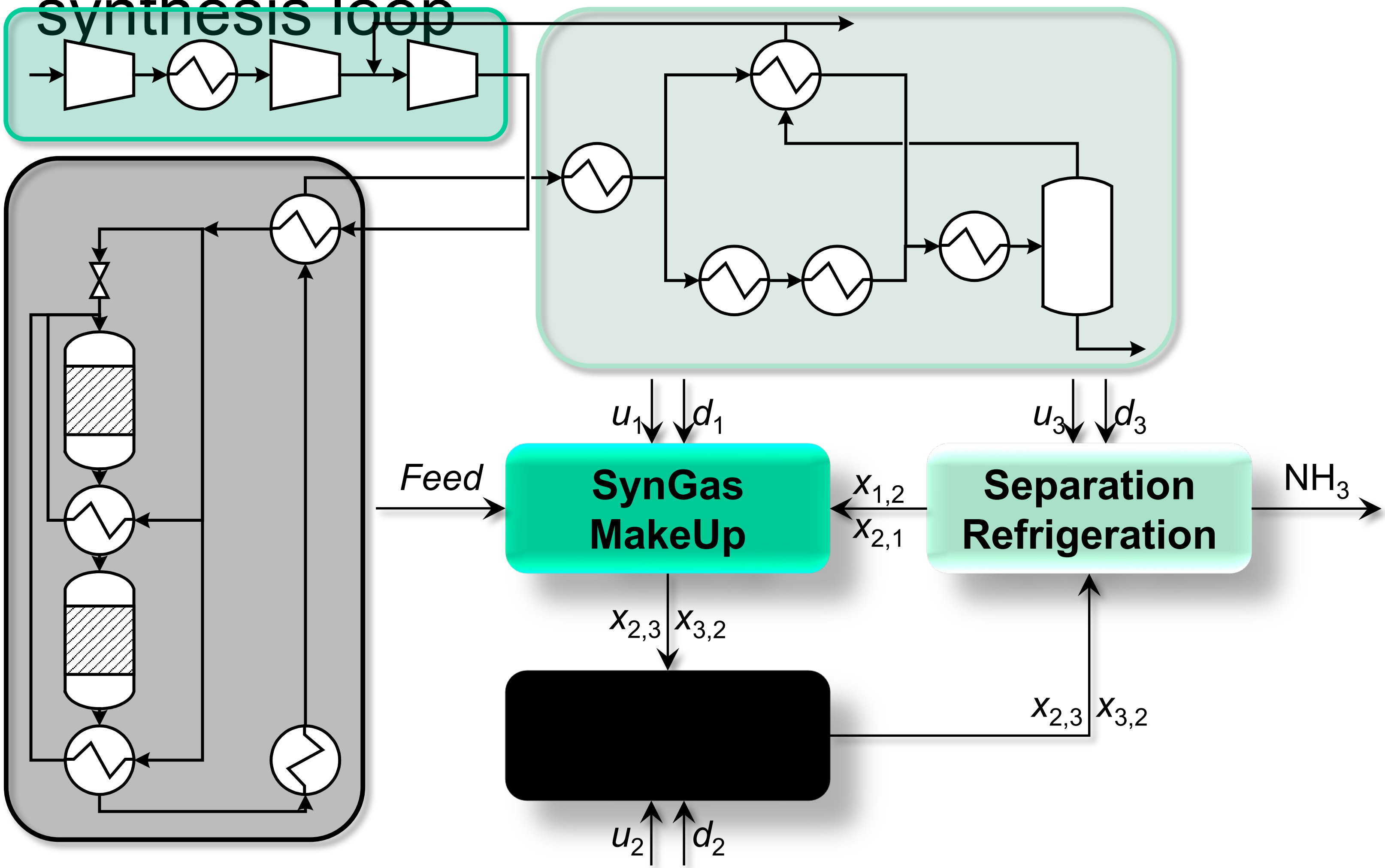
- Idea:
  1. Separate flowsheet into *n* independent submodels
  2. Define surrogate models for submodels
  3. Optimize new optimization problem

$$
\begin{aligned}
&\min_{u} J(x,u,d) \\
&\text{s.t. } f_i(x_i,u_i,d_i) = 0 \qquad\qquad (2) \\
&\qquad g_i(x_i,u_i,d_i) \leq 0
\end{aligned}
$$

- Requirement:
  - Introduction of new connection equality constraints:

$$
f_{i,j} = x_{i,j} - x_{j,i} = 0
$$

Example: Flowsheet separation – Ammonia synthesis loop

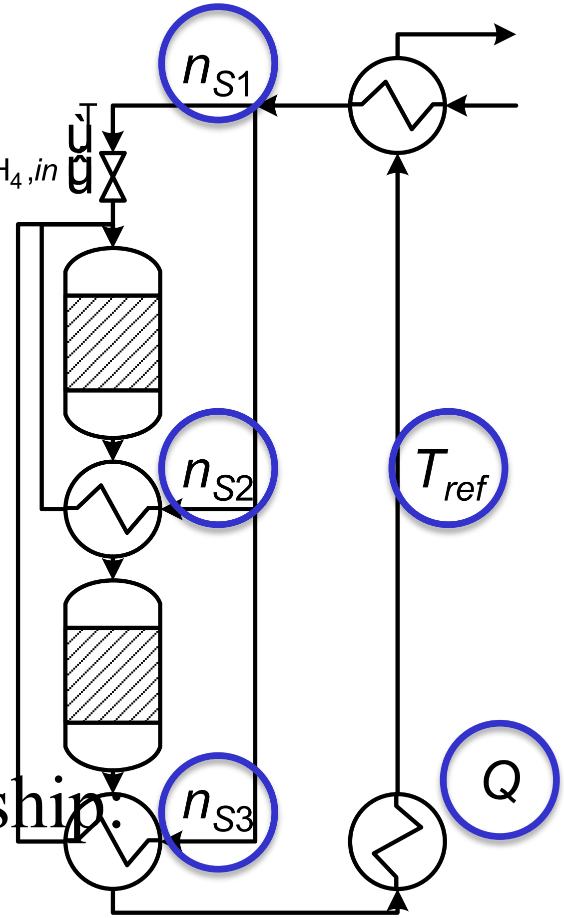


Example: Variable reduction – Reactor section

- Overall 10 independent variables:

$d = [p_{in} \quad T_{in} \quad n_{H_2,in} \quad n_{N_2,in} \quad n_{NH_3,in} \quad n_{Ar,in} \quad n_{CH_4,in}]^T$

$u = [n_{S1} \quad n_{S2} \quad Q]^T$



- Variable transformation:
  - $u = [n_{S1} \quad n_{S2} \quad T_{ref}]^T$

Reduce no. of variables:

1. Linear Relationships:
   - Mass balances $n_{i,out} = n_{i,in} + n_i x$
2. Active constraints + relationship:
   - Non, limited feed ratios.

- Only 3 surrogate model outputs:
  - Variables x, p_{out}, T_{out}

More “focused” surrogate models by proper selection of independent variables.

- Surrogate model depends on independent variable selection
  1. Existing control structure
  2. Introduction of self-optimizing control variables

- Approaches for independent variable reduction:
  1. Linear relationships do not need surrogate models
  2. Active constraints as constants or disturbances
  3. Relationships between connected variables *e.g.* coming from reaction section shall be exploited. (Extent of reaction ξ)
  4. Dimensionless numbers based on physics or dimensions (Buckingham-Pi-theorem)

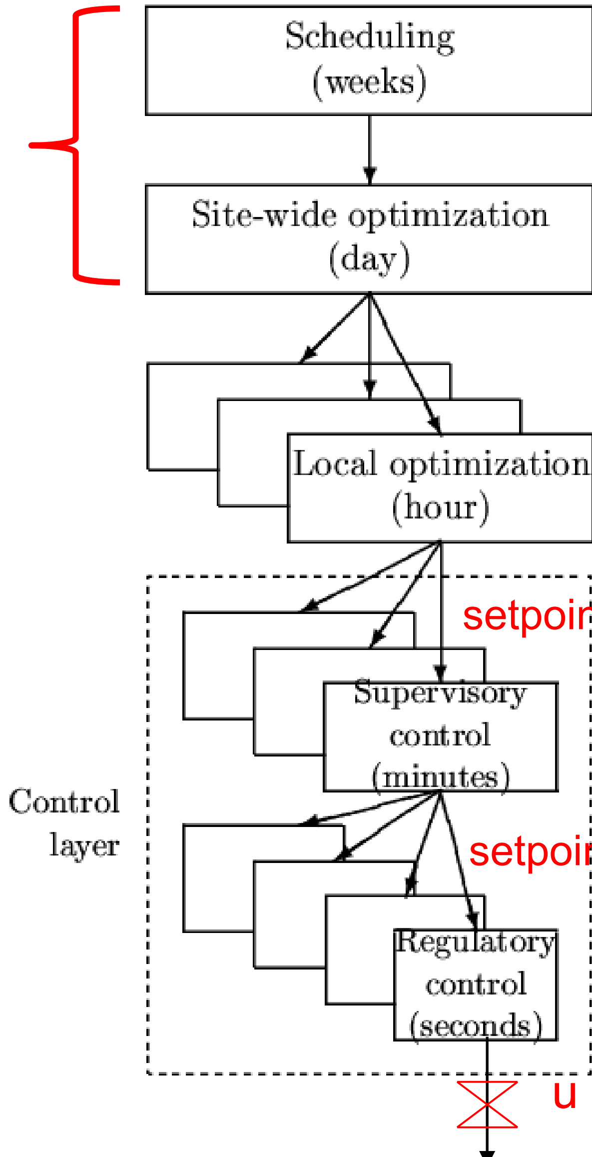
3. Planning challenges

- Sigurd on thin ice…. ☺

Our Paradigm

Decision hierarchy

Planning



Manager

Process engineer

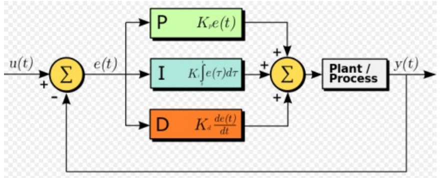
Operator/RTO

setpoints

Operator/"Advanced control"/MPC

setpoints

PID-control



u = valves

3. Planning challenges

- Control: one hour time scale
    - Control active constraints + self-optimizing variables
  - Must have detailed model of overall plant to identify optimal active constraints
- Planning: One day-week time scale
  - Usually have simplified models of units
  - Use: Max. Capacity of each unit and simple models for energy usage

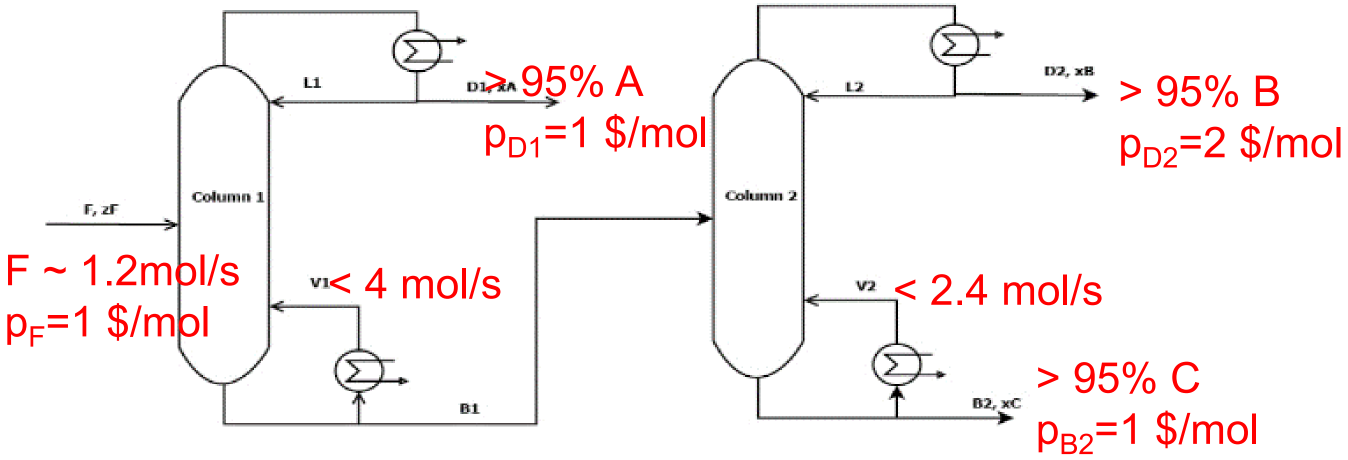
Planning

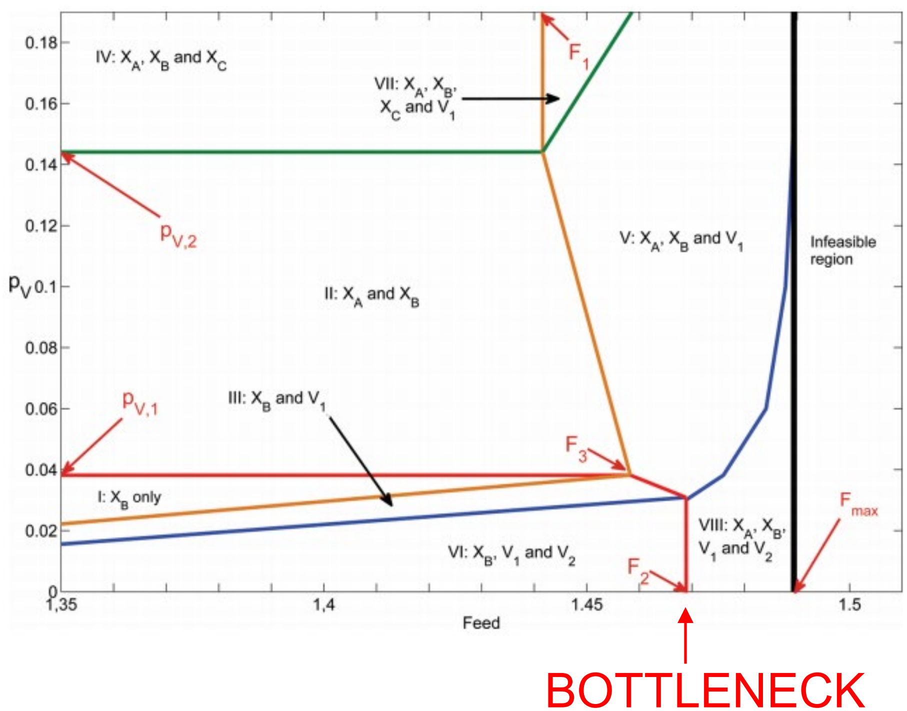
- Production optimization (day)
  - Stop/start of units / trains
  - Production rates (feeds to units, production rates)
  - Adjusted specifications = constraint values (purities)
  - Expected active constraints (max. flows, etc.)
- Scheduling (weeks)
  - Buying of raw material (feed amounts and feed specs)
  - Shipment of products
  - Planned maintenance
  - Uncertainty may be important -> Stochastic optimization

Question: How detailed models do we need for planning?

- To be truly optimal need full nonlinear model
- Refinery planning: Linear programming (LP) models used
  - Each unit: Lnear yield model + constraints (?)

Distillation columns in series: Planning



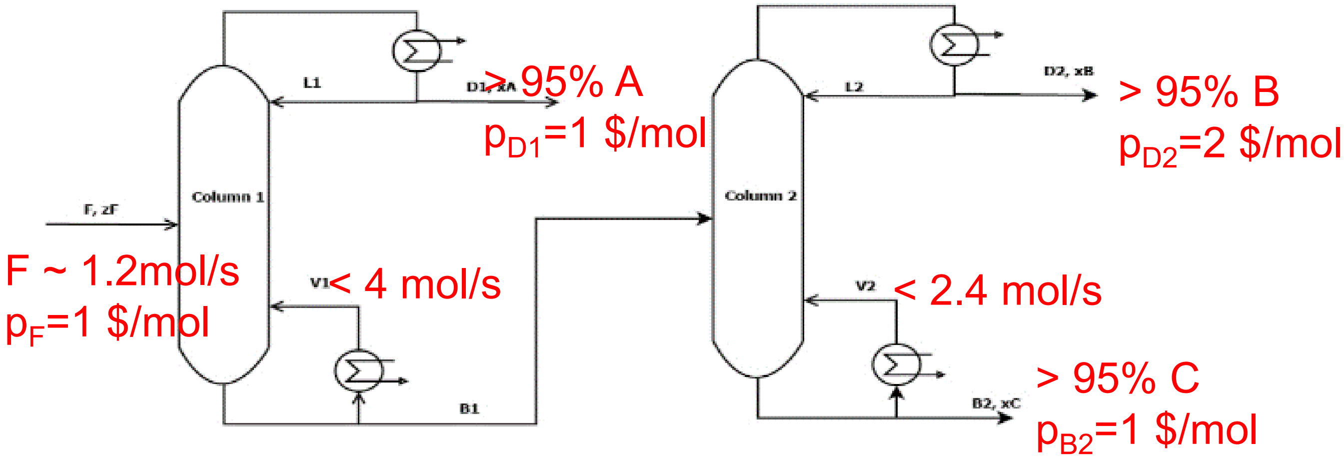


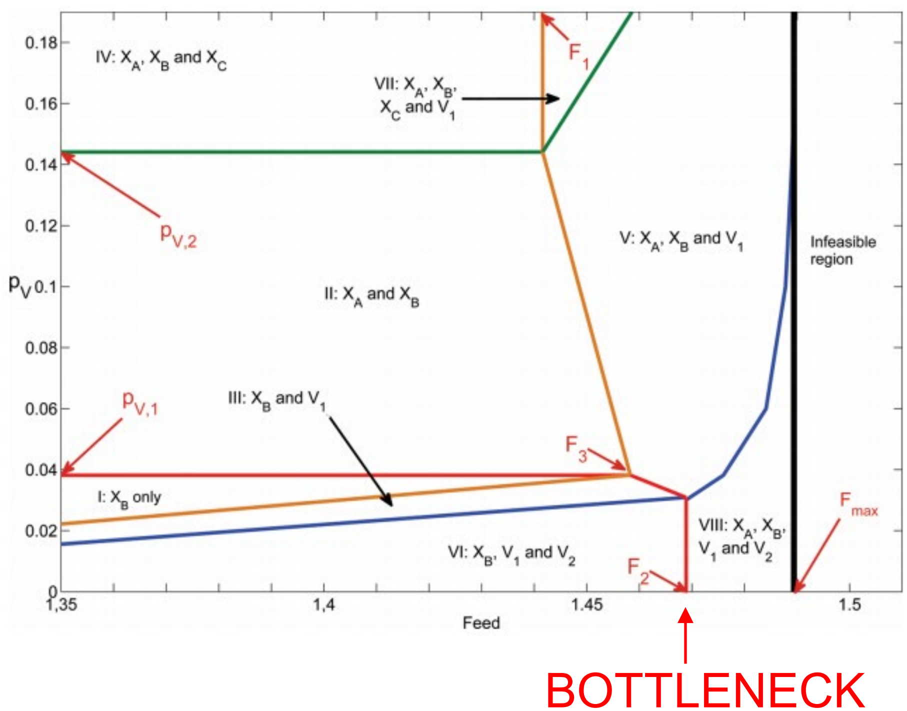
1. Daily optimization to decide on feedrate:

Would expect to operate at bottleneck (max. Feed =1.49) unnless:

1. Sellable product rates limited
   - D/F and B/F will depend somewhat on which other constraints are active
2. Available feed limited

Distillation columns in series: Planning





2. Longer term optimization to decide on: which feed to buy, product quality, etc

Could be uncertainty in future prices, shipping delays, etc.

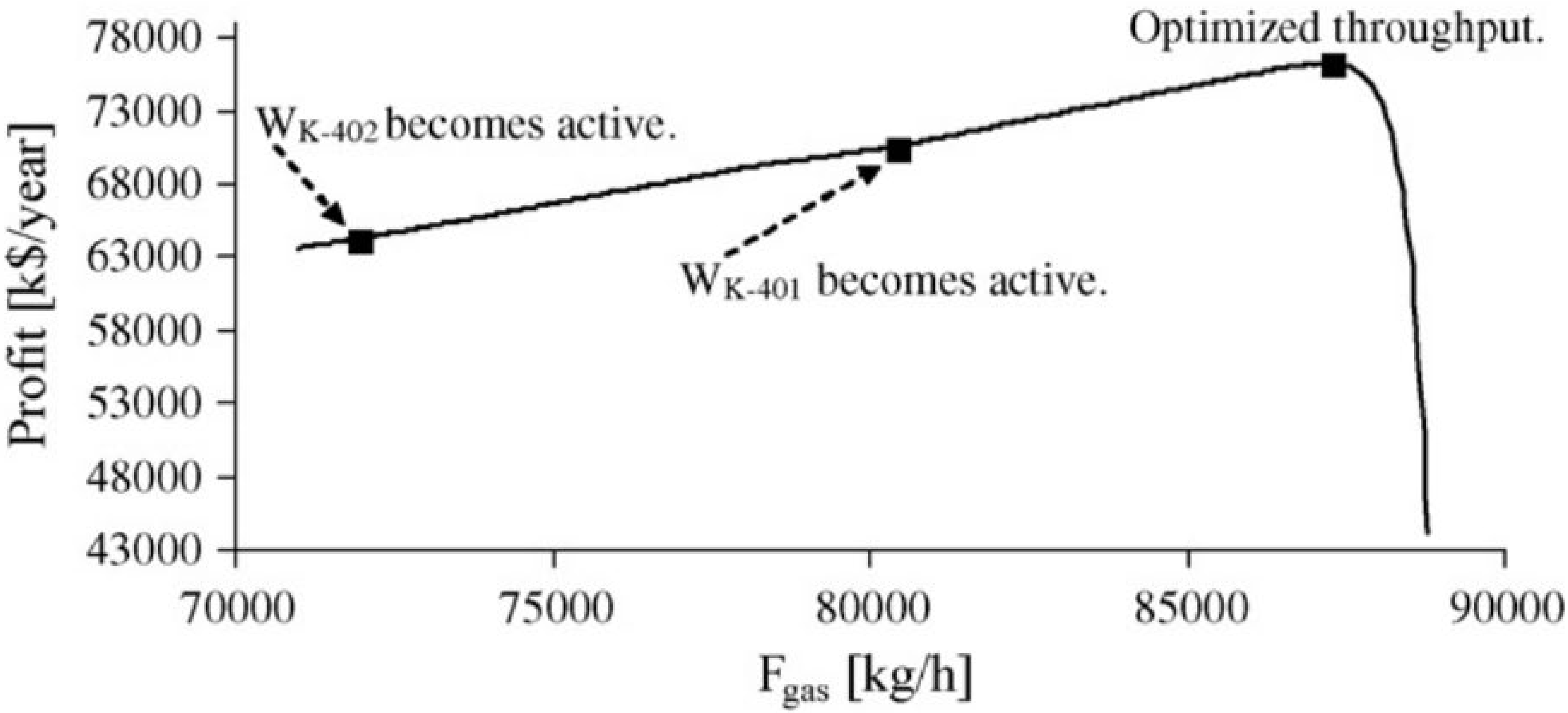


Fig. 3. Optimization of the ammonia plant with variable gas feed rate F_{gas}.

“Control structure design for the ammonia synthesis process”
Antonio Araujo, Sigurd Skogestad ∗Computers and Chemical Engineering 32 (2008) 2920–2932

Incorrect simplification. ΔTmin

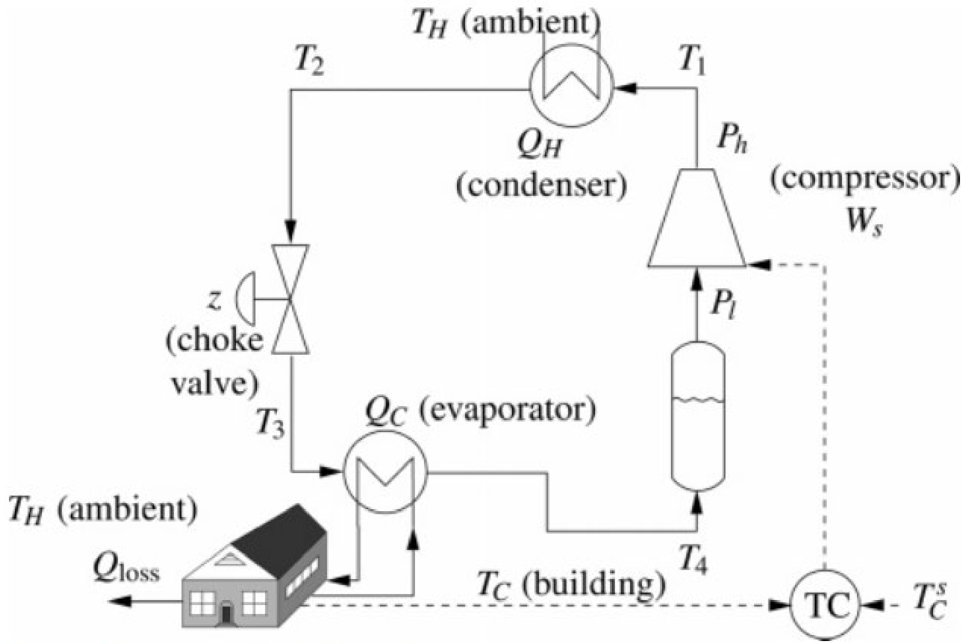
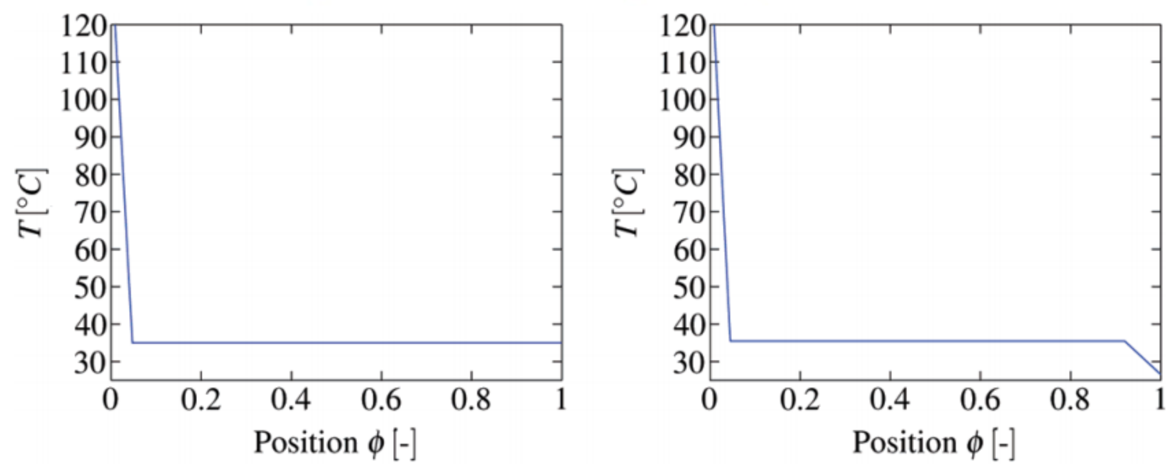


Figure 2. Ammonia refrigeration system.



(a) Optimal design with specified ΔT_{min}

(b) Re-optimized operation with specified A

“Problems with Specifying Dtmin in the Design of Processes with H

Optimal centralized Solution (EMPC)

Academic process control community fish pond