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Maryam GHADRDAN

October 24, 2014





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Thesis Contributions

Chapter 1 Introduction

Chapter 2 a short review on Thermally coupled columns, with focus on Kaibel columns, their design, optimal operation and control.

Chopter 3 Two operation modes

- maximizing the purities in the products with fixed boilup
- minimizing energy with specified product purities
- **Chapter 4** shortcut design of a Kaibel column using *V*_{min} diagram.
- Chopter 5 Vapour split as a degree of freedom. Two methods are used to study the effect of vapour split manipulation, namely a shortcut method and rigorous simulations.

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Chapter 6 short review of self-optimizing methods.



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Thesis Contributions

Chapter 7 Control of Kaibel columnfor the case of maximizing purities of products with fixed boilup.

Chapter 8 Short review on static estimators.

Chapter 9 A new class of static estimators for four different scenarios:

- open
- primary variables are controlled
- secondary variables are controlled
- estimation of primary variables are controlled.

Chapter 10 Control of Kaibel column for specified product composition

Chapter 11 Dynamic compensation for static estimators



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V_{min} diagram



Figure: V_{min} diagram for a ternary feed



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Figure: V_{min} diagram for the prefractionator of Kaibel distillation column (b/c split)





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V_{min} diagram for Kaibel distillation column







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Dynamic compensation of static estimators **Table:** Procedure of making the V_{min} diagrams from rigorous simulations

Line	Specifications
0 - a/b	$R_{C2,bot} = UB$, Increase D while $R_{C1,top} < UB$,
a/b - a/c	$R_{C1,top} = UB$, Increase D while $R_{C3,top} < LB$,
a/c - b/c	$R_{C3,bot} = UB$, Increase D while $R_{C2,top} < UB$
b/c - b/d	$R_{C2,top} = UB$, Increase D while $R_{C4,top} < LB$
b/d - c/d	$R_{C4,top} = UB$, Increase D while $R_{C3,top} < UB$
c/d - end	$R_{C3,top} = LB$, Increase D while $R_{C1,bot} < LB$
a/c - a/d	$R_{C1,top} = UB$, Increase D while $R_{C4,top} < LB$
a/d - b/d	$R_{C4,bot} = UB$, Increase D while $R_{C2,top} < UB$





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V_{min} from rigorous simulation





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Definition of the Objective Function

Two different ways to operate a column:

- Mode 1 Specify the product purities and use the remaining DOF for minimizing the vapor consumption (motivation to introduce thermally-coupled columns)
- Mode 2 Fix the column boilup at the maximum and try to get the most out of the column (when energy is relatively cheap)





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Figure: Simulation flowsheet of Kaibel distillation column



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Mode 1

The optimal values are obtained by plotting the contours manually.





Figure: Contours of constant boilup as a function of vapour and liquid splits at constant product purities

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Mode 1



Figure: (Left) Boilup rate as a function of liquid split at constant vapour split and product purities, (Right) Impurities in the top and bottom of prefractionator





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Multiplicity is seen in the

solution

Obs!



Figure: Paths of impurity flow to side streams







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Mode 1: Impurities along a boilup contour

0.06





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C2 in Pref. Bot. C3 in Pref. Top

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Mode 2:

Objective J is to minimize the loss compared to the ideal profit (pure products).

$$J = D(1 - x_D) + S_1(1 - x_{S1}) + S_2(1 - x_{S2}) + B(1 - x_B)$$

DoF $u = \begin{bmatrix} R_L & R_V & L & S_1 & S_2 \end{bmatrix}$

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Optimization is done in MATLAB using GA method







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Mode 2



Figure: Mode 2 with fixed boilup: 3-D surfaces and contour plot of impurity sum (cost J) as a function of degrees of freedom with the other variables fixed at their optimal values.

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 $R_V = R_{V,nom}$?

 V_{min} diagram for the nominal feed properties (black) and new feed composition with optimal (blue) and fixed R_V (red)



Figure: b/c composition change from 0.25/0.25 to 0.30/0.20 with optimal $R_V = 0.5649$ and fixed $R_V = 0.5846$



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 $R_V = R_{V,nom}$?



Change in a/b composition



Change in c/d composition



Change in b/c composition

Contours of boilups up to 2% more than minimum energy for different feed composition changes in A/B, B/C and C/D

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Comparison of energy saving for two different vapour split values

Compositions	(x_a/x_b)		(x_b/x_c)		(x_c/x_d)	
	R _{V,nom}	R _{V,lower}	R _{V,nom}	R _{V,lower}	R _{V,nom}	R _{V,lower}
0.1/0.4	0.8%	2.7%	14.2%	8.67%	2.7%	-0.02%
0.15 / 0.35	0.07%	1.41%	6.96%	2%	0.65%	0.5%
0.2 / 0.3	0%	0.96%	0.8%	0.05%	0%	0.97%
0.3 / 0.2	0%	1.1%	0.85%	0.33%	0%	0.67%
0.35 / 0.15	0%	1.12%	3.58%	0.16%	0%	0.68%
0.4 / 0.1	0%	0.8%	6.54%	6.98%	0.5%	1.9%







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General procedure for control structure design

I Top-down (focus on steady-state economics)

- Define operational objectives (optimal operation):
 - Cost function J (to be minimized)
 - Constraints
- Objective: Find regions of active constraints
 - Identify steady-state DOF
 - expected disturbances.
 - Optimize the operation wrt the DOF for the expected disturbances (off-line analysis)
 - Select primary controlled variables CV1s (Self-optimizing)





Select location of throughput manipulator





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II Bottom-up (focus on dynamics)¹

- Select structure of regulatory control layer (including inventory control):
 - Select 'stabilizing' controlled variables CV2
 - Select inputs (valves) and 'pairings' for controlling CV2 (Decision 4)
 - Stabilizes the process and avoids drift
 - ② If possible, use same regulatory layer for all regions
- Select structure of supervisory control
 - Controls primary CV1's
 - Supervises regulatory layer
 - Performs switching between CV1s for different regions
- Select structure of (or need for) optimization layer (RTO)
 - Updates setpoints for CV1 (if necessary)

¹Skogestad, S., 2004, Control Structure Design for Complete Chemical Plants, Computers and Chemical Engineering, 28, 219-234



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Loss Method

OBJECTIVE

Self-optimizing control is when we can achieve an acceptable loss with constant setpoint values, for the controlled variables in the presence of disturbance and noise.

2

$$\mathsf{L}(\mathsf{H}, d, e) = \mathsf{J}(u, d, e^{x})_{c=c^{*}} - \mathsf{J}(u^{\textit{opt}}(d), d)$$

where d and e are constrained to satisfy the following inequality

$$\| \begin{bmatrix} d' & n^x \end{bmatrix}^T \|_2 \le 1$$

and $d = \mathbf{W}_d d'$ and $n^x = \mathbf{W}_{n^x} n^{x'}$.

²Skogestad, S. (2000). Plantwide control: The search for the self-optimizing control structure. Journal of Process Control 10, 487-507



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Assumption: Linear steady-state measurement model,

 $\mathbf{x} = \mathbf{G}_{\mathbf{x}}\mathbf{u} + \mathbf{G}_{\mathbf{x}}^{d}\mathbf{d}$

The actual measurements \mathbf{x}_m , containing noise \mathbf{n}^x is

$$\mathbf{x}_m = \mathbf{x} + \mathbf{n}^x$$

The CVs of the form
$$\mathrm{c}=\mathsf{H}\mathrm{x}_m$$

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$$\min_{\mathbf{H}} \|\mathbf{J}_{uu}^{1/2} (\mathbf{H}\mathbf{G}_x)^{-1} \mathbf{H}\tilde{\mathbf{F}}\|_F^2$$

where $\tilde{\mathbf{F}} = \begin{bmatrix} \mathbf{F} \mathbf{W}_d & \mathbf{W}_{n^x} \end{bmatrix}$.

F: optimal sensitivity matrix. It can be found

• using
$$\mathbf{F} = -\mathbf{G}_x \mathbf{J}_{uu}^{-1} \mathbf{J}_{ud} + \mathbf{G}_x^d$$

• numerically from its definition $\mathbf{F} = \frac{dy_{opt}}{dd}$ \checkmark

J_{uu} can be difficult to obtain, especially if one relies on numerical methods, and also taking the difference can introduce numerical inaccuracy.





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Mode 2; Control Structure design

- 5 steady-state DOF: reflux rate, side stream flows, liquid split and vapor split
- Need to find 5 CVs: Single temperatures
- Throughput Manipulator (TPM): column feed
- Assumed that the temperature loops in the upper layer are used for stabilization too
- Disturbances: feed flow rate (*F*), feed composition (*z_F*) and feed liquid fraction (*q*), setpoints of controllers.





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Optimal Profiles in Kaibel Arrangement



Optimal composition (left) and temperature (right) profiles



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Figure: Optimal temperature profiles for disturbances in feed compositions, liquid fraction and boilup flow setpoint





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Pairings

- Avoid pairing on negative steady-state RGA
- Choose pairings corresponding to RGA-elements close to 1
- Prefer pairing on variables with good controllability (=small effective delay).

$$RGA(\mathbf{G}) = \mathbf{G} \times (\mathbf{G}^{-1})^T$$

	R_l	R_{v}	RR	Side ₁	Side ₂	
<i>T</i> 15	0.31	0.72	0.49	-0.06	-0.47	1
<i>T</i> 36	-0.74	0.42	10.37	0.33	-9.38	
<i>T</i> 39	2.18	-0.78	4.16	-1.50	-3.07	
<i>T</i> 54	-1.13	0.77	-4.22	2.31	3.27	
<i>T</i> 75	0.38	-0.13	-9.81	-0.08	10.64	



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Our Static Estimator

OBJECTIVE

The main objective is to find a linear combination of measurements such that keeping these constant indirectly leads to nearly accurate estimation with a small loss L in spite of unknown disturbances, d, and measurement noise, n^x .

$$\min_{\mathbf{H}} \left\| \boldsymbol{e} \right\|_{2} = \left\| \mathbf{y} - \hat{\mathbf{y}} \right\|_{2}$$





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Our Static Estimator

- "Open-loop" (for Monitoring of ŷ)
 - No control (u is a free variable)
 - Primary variables y are controlled (u is used to keep y = y_s).
 - Secondary variables z are controlled (u is used to keep z = z_s).
- "Closed-loop" (for Control of ŷ)













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Our Static Estimator



 Assumption: Linear models for the primary variables y, measurements x, and secondary variables z

 $\mathbf{y} = \mathbf{G}_{\mathbf{y}}\mathbf{u} + \mathbf{G}_{\mathbf{y}}^{d}\mathbf{d}$ $\mathbf{x} = \mathbf{G}_{\mathbf{x}}\mathbf{u} + \mathbf{G}_{\mathbf{x}}^{d}\mathbf{d}$ $\mathbf{z} = \mathbf{G}_{\mathbf{z}}\mathbf{u} + \mathbf{G}_{\mathbf{z}}^{d}\mathbf{d}$

$$\mathbf{G}_{\gamma} = \left(\frac{\partial y}{\partial u}\right)_{d}, \mathbf{G}_{\gamma}^{d} = \left(\frac{\partial y}{\partial d}\right)_{u}, \cdots$$

- **2** The actual measurements x_m , containing measurement noise n^x is $x_m = x + n^x$
- **③** The linear estimator is of the form $\hat{y} = Hx_m$

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Optimal estimators for different scenarios

"Open-loop" 1 $H_{1} = Y_{1}X_{1}^{\dagger}$ $Y_{1} = \begin{bmatrix} \mathbf{G}_{y}\mathbf{W}_{u} & \mathbf{G}_{y}^{d}\mathbf{W}_{d} & \mathbf{0} \end{bmatrix}$ $Y_{2} = \begin{bmatrix} \mathbf{W}_{y_{s}} & \mathbf{0} & \mathbf{0} \end{bmatrix}$ $X_{1} = \begin{bmatrix} \mathbf{G}_{x}\mathbf{W}_{u} & \mathbf{G}_{x}^{d}\mathbf{W}_{d} & \mathbf{W}_{n^{x}} \end{bmatrix}$ $X_{2} = \begin{bmatrix} \mathbf{G}_{x}^{cl}\mathbf{W}_{y_{s}} & \mathbf{F}\mathbf{W}_{d} & \mathbf{W}_{n^{x}} \end{bmatrix}$

"Open-loop" 3

 $\mathbf{Y}_3 = \begin{bmatrix} \mathbf{G}_y^{cl} \\ \mathbf{X}_3 \end{bmatrix} \mathbf{G}_y^{cl} \mathbf{V}_y$

"Closed-loop"

$$\begin{aligned} \mathbf{H}_{3} &= \mathbf{Y}_{3} \mathbf{X}_{3}^{\dagger} & \min_{\mathbf{H}} \left\| \mathbf{H} \left[\mathbf{F} \mathbf{W}_{d} \quad \mathbf{W}_{n^{x}} \right] \right\|_{I} \\ \mathbf{W}_{z_{s}} \quad \mathbf{F}_{y}^{\prime} \mathbf{W}_{d} \quad \mathbf{O} \end{array} \right] & \text{s.t. } \mathbf{H} \mathbf{G}_{x} = \mathbf{G}_{y} \\ \mathbf{V}_{z_{s}} \quad \mathbf{F}_{x}^{\prime} \mathbf{W}_{d} \quad \mathbf{W}_{n^{x}} \end{aligned}$$



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Open-loop estimation (S1)



Figure: Top estimate with -1 percent change in boilup

Figure: Bot estimate with -1 percent change in boilup



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Open-loop estimation (S3)





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OL estimation (S3) (contd.)





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Closed-loop estimation (S4)





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Closed-loop estimation (S4)



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Improving dynamic performance

The fast dynamics of measurements with negative contributions may lead to inverse response (RHP zero in the transfer function from u to CV)

• Cascade Control:

Close a fast inner loop and adjust the setpoint on a time scale which is slower than the RHP-zero.

• Use of measurements from the same section of the process:

Selected measurements are similar, then it is less likely to get RHP-zero. However, this gives a larger steady-state error.

• Filters:

The Low-pass filters will keep the system optimal at steady state.



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Example

G

$$\mathbf{G}_{x} = \begin{bmatrix} \frac{1}{3s+1} \\ \frac{1}{s+1} \end{bmatrix}$$

and the optimal matrix **H** is

 $\mathbf{H} = \left[\begin{array}{cc} \mathbf{2} & -\mathbf{1} \end{array} \right]$

the transfer function from \boldsymbol{u} to $\hat{\boldsymbol{y}}$ is

$$= HG_{x} = \frac{2}{3s+1} - \frac{1}{s+1} = \frac{1-s}{(3s+1)(s+1)} \approx \frac{e^{-1.5s}}{3.5s+1}$$

Figure: Block diagram of the estimation

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Cascade (inner-loop) can not move the zero of **HG**_{*x*}

Proof.

Theorem



By performing the loop calculations, the transfer function from x_{2s} to \hat{y} is

$$\hat{\mathbf{y}} = (h_2 + h_1 \frac{g_1}{g_2}) \frac{kg_2}{1 + kg_2} x_{2s} \tag{1}$$

The term $(h_1g_1 + h_2g_2)$, which includes the RHP zero, is unchanged.

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Figure: Block diagram of the estimation system including filter (H_F)

$$\mathbf{H}_{F} = \begin{bmatrix} \frac{1}{\tau_{F_{1}s+1}} & \mathbf{0} \\ \mathbf{0} & \frac{1}{\tau_{F_{2}s+1}} \end{bmatrix}$$
$$\mathbf{H}_{F}(\mathbf{0}) = I$$



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Some Filters:

$$\mathbf{H}_{F1} = \begin{bmatrix} \frac{1}{s+1} & \mathbf{0} \\ \mathbf{0} & \frac{1}{3s+1} \end{bmatrix}$$

$$\mathbf{H}_{F2} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{s+1}{3s+1} \end{bmatrix}$$



	1	0	1
$\mathbf{n}_{F4} =$	0	$\frac{1}{3s+1}$	

The filtered transfer function will be

$$\mathbf{H}_{dyn1}\mathbf{G}_{x} = \frac{1}{(3s+1)(s+1)}$$

$$\mathbf{H}_{dyn2}\mathbf{G}_{x} = \frac{1}{3s+1}$$

$$\mathbf{H}_{dyn3}\mathbf{G}_{x}=\frac{1}{s+1}$$

$$H_{dyn4}G_x = \frac{2s+1}{(3s+1)(s+1)}$$

Using Lead-lag compensators, we can make the response as fast as we want.



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Distillation case-study



Figure: $HG_x(t)$ with -1% change in **Figure:** Estimated composition (tf boilup and constant Reflux ratio = HG_x) and filtered estimated compacities (tf = HH_xG_x) where

composition (tf = HH_FG_x) where there are filters only on 6th, 16th and 17th measurements



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Optimizing filters





Figure: Real composition, Estimated composition (tf = HG_x) and filtered estimated composition (tf = HH_FG_x) where filters are optimized for first 100 min. assuming $G_{ref} = G_{u \rightarrow y_1}$

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Explicit solution for the filter problem

Approach:

Convert the model matching problem to Nehari problem

$$\|\mathbf{T}_1 - \mathbf{T}_2 \mathbf{Q} \mathbf{T}_3\|_{\infty} \ \Rightarrow \ \|\mathbf{R} - \mathbf{X}\|_{\infty} = \|\boldsymbol{\Gamma}_R\|$$

- In our case we have $T_3 = I$
- An optimal Q exists if the ranks of the two matrices
 T₂(jω) and T₃(jω) are constant for all 0 < ω < ∞³.
- ³Francis1987.



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Scalar-valued case

Step 1Perform inner-outer factorization for T_2 Step 2R = [A, B, C, 0] (A antistable) + R_2 (in RH_{∞})Step 3The controllability and observability grammians are
the solutions of

$$AL_{c} + L_{c}A^{T} = BB^{T}$$
$$A^{T}L_{o} + L_{o}A = C^{T}C$$

Step 4 Having λ^2 =largest eigenvalue of $L_c L_o$ and the corresponding eigenvector (ω), define

$$f(s) := [A, \omega, C, 0]$$
$$g(s) := [-A^{T}, \lambda^{-1}L_{o}\omega, B^{T}, 0]$$

Step 5 $X = R - \lambda \frac{f}{g}$
Step 6 $Q = \mathbf{T}_{2o}^{-1}X$



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Example

In our example, we have the following inputs:

$$T_{1} = \frac{1}{0.5s + 1}$$
: Desired transfer function (G_{ref})
$$T_{2} = \frac{-s + 1}{3s^{2} + 4s + 1}$$
Current transfer function (HG_{x})

Since the rank of T_2 is not constant for all $0 \leq \omega \leq \infty,$ a transfer function

$$\mathbf{V} = (s+1)^{l}$$
$$\mathbf{Q} = \frac{19.82s^{2} + 2042s + 678.5}{s^{2} + 1002s + 2000}$$





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Matrix-valued case

The general algorithm to obtain **Q** is as follows **Step 1** Find a minimal realization of **R**: $\mathbf{R}(s) = [\mathbf{A}, \mathbf{B}, \mathbf{C}, 0]$ **Step 2** Solve the Lyapunov equations to find controllability and observability gramians and set $\mathbf{N} = (\mathbf{I} - \mathbf{L}_o \mathbf{L}_c)^{-1}$ **Step 3** Set

$$\begin{aligned} \mathbf{L}_{1}(s) &= \begin{bmatrix} \mathbf{A} & -\mathbf{L}_{c}\mathbf{N}\mathbf{C}^{T} & \mathbf{C} & \mathbf{I} \end{bmatrix} \\ \mathbf{L}_{2}(s) &= \begin{bmatrix} \mathbf{A} & \mathbf{N}^{T}\mathbf{B} & \mathbf{C} & \mathbf{0} \end{bmatrix} \\ \mathbf{L}_{3}(s) &= \begin{bmatrix} -\mathbf{A}^{T} & \mathbf{N}\mathbf{C}^{T} & -\mathbf{B}^{T} & \mathbf{0} \\ \mathbf{L}_{4}(s) &= \begin{bmatrix} -\mathbf{A}^{T} & \mathbf{N}\mathbf{L}_{o}\mathbf{B}^{T} & \mathbf{B}^{T} & \mathbf{I} \end{bmatrix} \end{aligned}$$

 $\begin{array}{ll} \mbox{Step 4} & \mbox{Select } Y \mbox{ in } \textit{RH}_{\infty} \mbox{ with } \|Y\|_{\infty} \leq 1 \mbox{ (for example } Y=0) \\ & \mbox{ and set } X = R - \big(L_1Y + L_2\big) \big(L_3Y + L_4\big) \end{array}$

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Concluding Remarks

- Kaibel distillation columns can save operational costs if operated optimally
- *V_{min}* diagrams are very useful tools for design, analysis and operation of columns
- It's important to control the key component flows out of the prefractionator
- Combination of measurement will result in lower estimation error compared to using single measurements
- It's possible to have dynamic issues in the estimators which stems from combining measurements from different sections
- Dynamic issues can be alleviated by cascade control, combining subset of measurements or applying filters



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Dynamic compensation of static estimators Thanks for your attention

I believe that you can keep going long after you think you can't



