



## Dynamic Effects of Diabatization in Distillation Columns

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# Presentation Outline

Motivation

Introduction

Methodology

Dynamic Modeling

Simulation Study

Results

Conclusion

Future Work

# Motivation

- Increasing focus on environmental issues and resource management
- Distillation is a widely used separation process in the industry, but it is highly energy intensive. Some key numbers for USA in 1988:
  - Distillation accounted for 4% of the total energy consumption <sup>1</sup>
  - Roughly 40% of the processing energy used in refining and continuous chemical processes was used for distillation
- Conventional distillation columns operate at low efficiencies <sup>2</sup>
- Diabatic distillation columns **can** provide:
  - Higher efficiencies <sup>3</sup>
  - Less utilities and thus less operation cost <sup>4</sup>

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<sup>1</sup> Humphrey, J.L. et al., Separation process technology, McGraw-Hill, 1997

<sup>2</sup> de Koeijer, G. et al., 2000, Int. J. Applied Thermodynamics 3(3):105–110

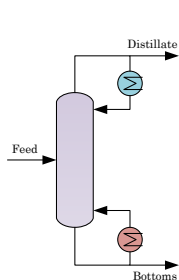
<sup>3</sup> Nakaiwa, M. et al., 1998, Appl. Therm. Eng., 18(11), 1077–1087

<sup>4</sup> Olujic, Z. et al., 2003, J. Chem. Technol. Biotechnol. 78(2-3):241–248

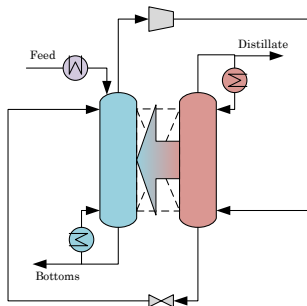
# Introduction

(1/3)

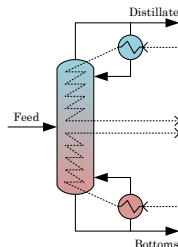
- **Adiabatic operation:** Heat is added at the highest temperature (reboiler) and heat is removed at the lowest temperature (condenser), thereby preventing integration (e.g. conventional,...)
- **Diabatic operation:** Heat required to perform the separation is added and/or removed throughout the column (e.g. HIDiC, DSHE, ...)



CDiC



General HIDiC



DSHE

# Introduction

(2/3)

- **Research example:** Verification of high heat transfer performance and enhanced mass transfer performance in a pilot scale (0,8 m diameter) test unit at TU Delft <sup>5</sup>



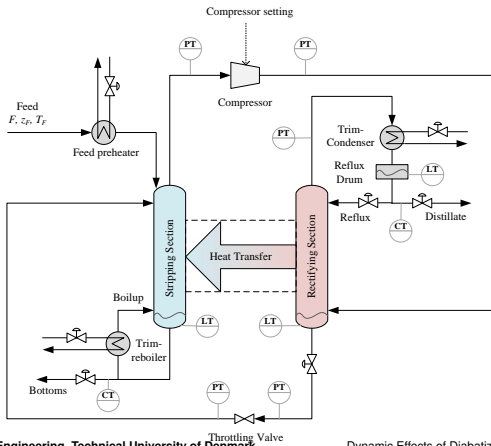
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<sup>5</sup><http://www.ecn.nl>

# Introduction

(3/3)

## The Heat-Integrated Distillation Column (HIDiC)



**CT:** Composition Transmitter

**LT:** Level Transmitter

**PT:** Pressure Transmitter

# Methodology

- Formulate generic, dynamic first-principle model describing:
  - Adiabatic distillation columns (Conventional)
  - Diabatic distillation columns (HIDiC)
- Implement model in simulator (Matlab<sup>®</sup>)
- Formulate realistic case-studies and perform numerical simulations
- Dynamic controllability analysis and compare distillation control configurations on decentralized  $2 \times 2$  system (remaining perfectly controlled)
- Perform closed-loop simulations based on single-loop control strategies



# Dynamic Modeling

- Model features:
  - Binary separation of benzene-toluene with **equally sized** rectifying and stripping section
  - **Mass balances**
  - **Energy balances**
  - Liquid tray hydraulics (variable liquid tray holdups)
  - One mathematical term distinguishes configuration (adiabatic, diabatic)
- Major assumptions:
  - Equilibrium stage model
  - Lewis/Randall ideal mixture
  - **Constant pressure** in each section
  - Negligible vapor holdup compared to liquid holdup
  - Negligible changes in sensible heat
  - Homogeneous stages (ideally mixed)

## Simulation Study

- Considered distillation column configurations:
  - Conventional distillation column (CDiC)
  - Heat-Integrated Distillation Column (HIDiC)

### Selected model parameters:

Parameter	Value
<b>Top purity</b>	99% benzene
<b>Bottom purity</b>	95% toluene
Number of stages	20
Feed stage location	11
Feed flow	100 $\frac{\text{kmol}}{\text{h}}$
Feed benzene content	0.50
Stripping section pressure	0.1013 MPa
Hydraulic time constant	0.0042 h
Heat of vaporization	30,001.1 $\frac{\text{kJ}}{\text{kmol}}$
<b>Relative volatility</b>	<b>2.317</b>
<b>Heat transfer rate</b>	<b>9,803 <math>\frac{\text{kJ}}{\text{h}\cdot\text{K}}</math></b>

# Results - Open-loop

(1/2)

Dynamic responses to step-changes in disturbance variables.

**Black curves:** +5%

**Gray curves:** -5%

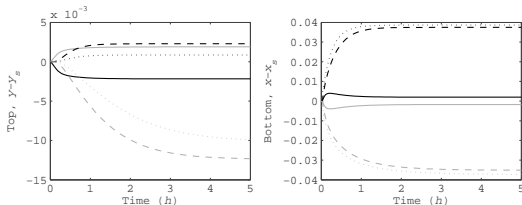
Legends:

**Dashed lines:** HIDiC

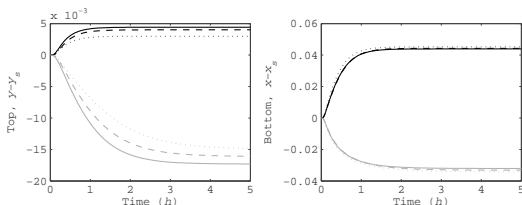
**Dotted lines:** CDiC

**(Solid lines:** HIDiC without condenser and reboiler)

Feed flow rate

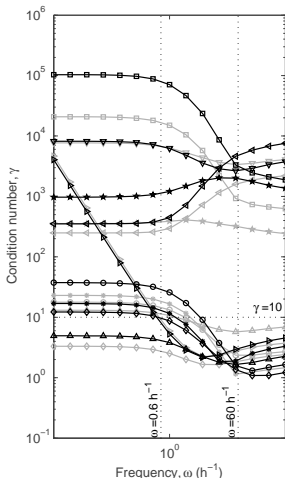
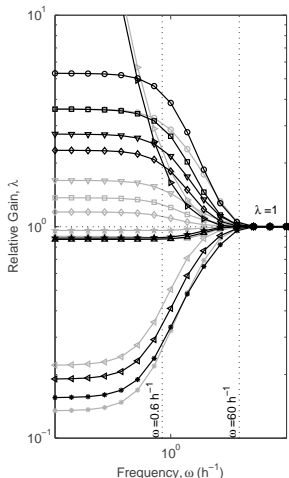


Feed composition



# Results - Open-loop

(2/2)



Controllability Analysis  
 Dynamic RGA Analysis and  
 SVA applied on a  
 decentralized  $2 \times 2$ :  
**HIDiC (black lines)**  
 and a  
**CDiC (gray lines)**.

**Legends:**

- (○): LV
- (\*) : DV
- (□): (L/D)V
- (△): LB ←
- (▽): L(V/B)
- (▷): DB
- (◁): D(V/B)
- (\*) : (L/D)B
- (◇): (L/D)(V/B)

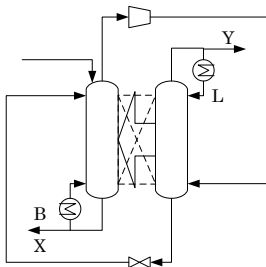
## Results - Closed-loop

(1/2)

- SISO controller based on an approximated First-order-Plus-Time-Delay model

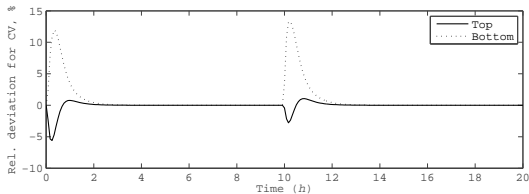
- Transfer function:

$$\begin{bmatrix} dY \\ dX \end{bmatrix} = \begin{bmatrix} \frac{-0.04972}{0.1336s + 1} \\ \frac{-0.009427}{0.055465s + 1} e^{-0.0897s} \end{bmatrix} \begin{bmatrix} \frac{-0.2566}{0.5070s + 1} e^{-0.0545s} \\ \frac{0.3144}{0.4357s + 1} \end{bmatrix} \begin{bmatrix} dL \\ dB \end{bmatrix}$$



## Results - Closed-loop

(2/2)



**Closed-loop responses** for the  
HIDiC to:

$t = 0$ h: +10% step-change in  
feed flow rate

$t = 15$ h: -10% step-change in  
feed composition

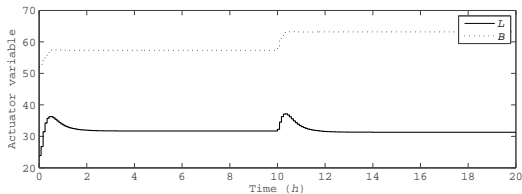
Tuning parameters (From S-IMC):

$dL \rightarrow dY_D$ :

$K_C = -0.0790$ ,  $\tau_I = 0.5158$ h

$dB \rightarrow X_B$ :

$K_C = 8.3147$ ,  $\tau_I = 0.4357$ h



## Conclusion

- A flexible and generic model have been developed to describe various diabatic distillation column configurations
- Various feasible pairings exist for the HIDiC
- Diabatization causes increased coupling between input-output variables
- In this study, among others an *LB*-structure seemed to be a promising control structure for a HIDiC

## Future Work

- PhD Project initiated with the title **Operation and Design of Diabatic Distillation Processes**
- Develop detailed model framework for adiabatic and diabatic distillation processes
- Investigations, including:
  - Thermodynamics: Impact on complex thermodynamic modeling on e.g. dynamics
  - Operability: Abnormal operation, e.g. steady-state multiplicity
  - Control: Development of regulatory and multivariable control strategies



**End**

Thank you for your attention