



# Validation and assessment of reduced models on an industrial distillation column

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[www.cybernetica.no](http://www.cybernetica.no)

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- Description of distillation column model
- Purpose of model reduction
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# Introduction to Cybernetica AS

## Model based control systems for the process industry



Cybernetica AS - [www.cybernetica.no](http://www.cybernetica.no)



## Background

- Founded in 2000
- At present 15 employees
- A spin-off company from the research groups in process control and engineering cybernetics at SINTEF, NTNU and Statoil



- Office in Trondheim, Norway

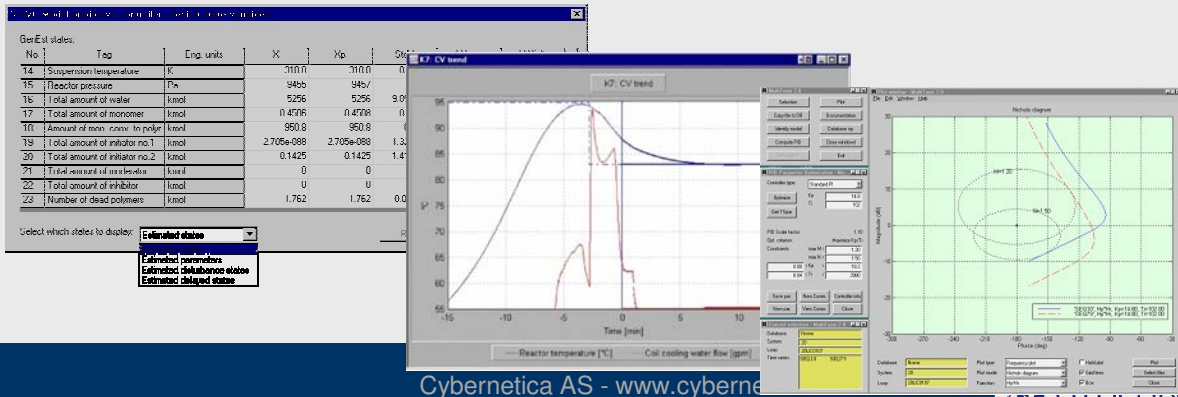
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# Products: Overview

- Model based control - Cybernetica CENIT
- Optimal grade transitions - Cybernetica CENIT
- Plant optimization - Cybernetica PlantOptimize
- Batch process optimization - Cybernetica BatchOptimize
- Controller tuning - Cybernetica MultiTune
- Dynamic simulation - Cybernetica SIMON



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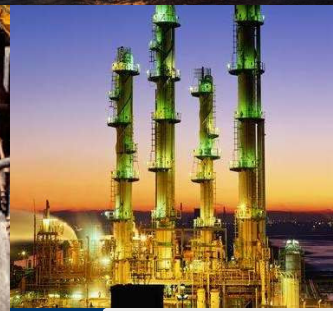
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# Applications: Overview

Polymer industry

Light metals

Oil and gas

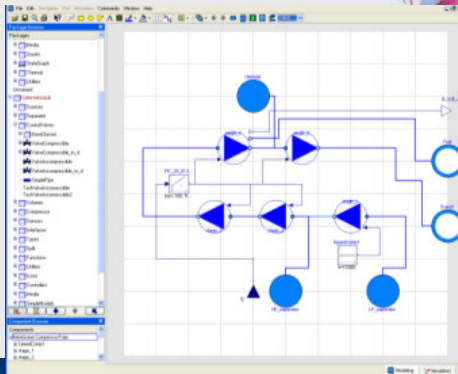
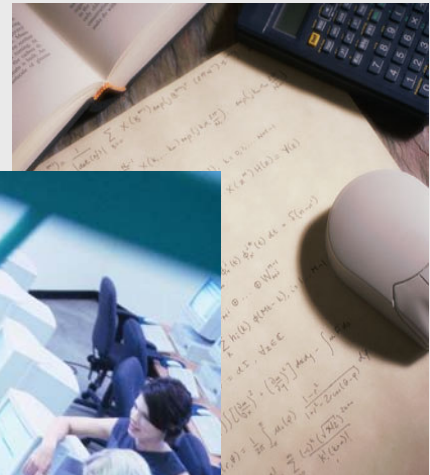


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- R&D projects



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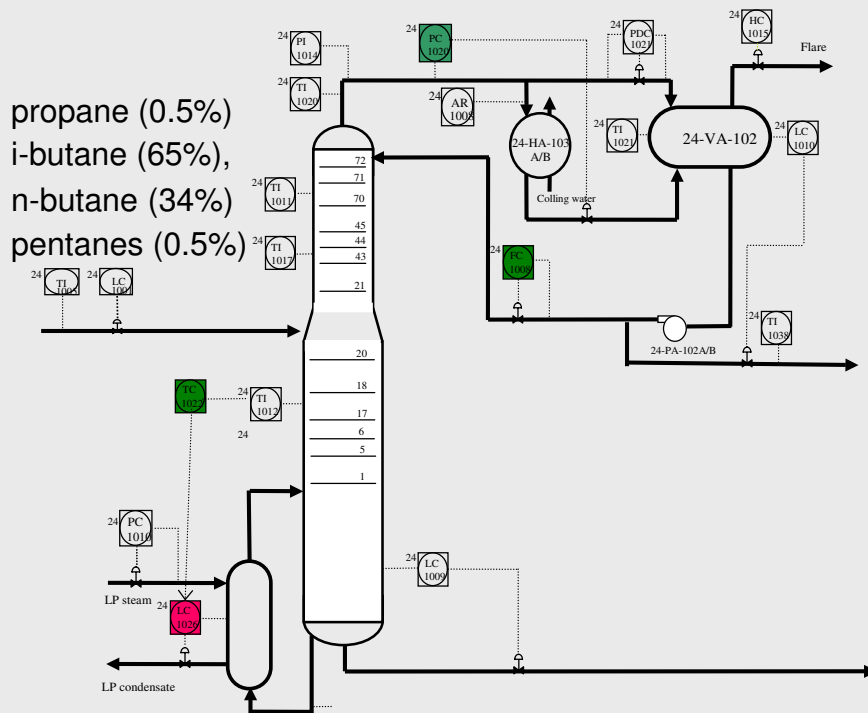
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# Description of distillation column model



Inputs for MPC:

- reflux rate
- temperature setpoint at 19th tray

Outputs for MPC:

- n-butane fraction at top
- i-butane fraction at bottom

## Model description

- mass balance per component for each tray, sump and reflux drum
- Energy balance for each tray, sump and reflux drum
- Complete flash at all trays, sump and in reflux drum.
- Vapour-liquid equilibrium is based on Soave-Redlich-Kwong equations

## Model description

- Vapour flow rates between trays depend on pressure differences between trays.
- Liquid flow rates between trays depend on liquid level on trays (weir equation)
- 4 PI controllers included in the model

## Summary of equations

474 differential equations, of the type :

$$\frac{dM_{k,i}}{dt} = L_{k-1}x_{k-1,i} + V_{k+1}y_{k+1,i} - L_kx_{k,i} - V_ky_{k,i} + \text{specific feeds for feed tray, sump and reflux drum}$$

$$\frac{dU_k}{dt} = L_{k-1}h_{k-1}^L + V_{k+1}h_{k+1}^V - L_kh_k^L - V_kh_k^V + \text{specific feeds for feed tray, sump and reflux drum}$$

k = tray number {1...94}

i = component number {1,2,3,4}

# Summary of equations

Outputs of the model:  $x, y, T, P$ , levels in sump and refluxdrum

$$[L, V, x, y, h, T, P, \text{levels}]^T = g(M, U)$$

$g(M, U)$  contains 188 implicit (non)linear algebraic equations ,  
e.g. SRK-equations

**Conclusion:** Many equations have to be integrated and solved using DAE-solvers, which leads to high computational loads

# Purpose of model reduction

Equations used in a distillation model and its application:

474 differential equations:  $\frac{dx}{dt} = f(x, z, u, d)$

188 algebraic equations:  $0 = g(x, z, u, d)$

2 output equations:  $y = h(x, z, d)$

Application: compute optimal input trajectories  $u$  with MPC

**Problem: Computation of  $u$  is too slow for fluctuations in  $d$ .**

**This leads to sub-optimal values for  $u$ .**

**Cause: Computation and use of large Jacobian:**

$$\begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial z} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial z} \end{bmatrix}$$

# Reduction methods and reduced models

Two used methods:

1. Tray aggregation (Andreas Linhart)
2. POD-grey box modeling (Reinout Romijn)

## Tray aggregation

**Reduction of number of state and algebraic equations:**

**Step 1:** Reducing number of state equations ( $f$ ), which leads to new state equations ( $f_1$ ) and new implicit algebraic equations ( $f_2$ ).

**Step 2:** Reducing number of implicit algebraic equations ( $f_2$  and  $g$ ), including those created in step 1 by calling for their solutions that are stored in tables.

**Step 3:** Efficient computation and storage of non-zero Jacobian elements for system that is obtained with steps 1 and 2.

Result (Linhart): reduced model is 6 times faster than full model at accuracies that are dominated by simulation errors.



# Tray aggregation

original model

$$\frac{dx}{dt} = f(x, z, u, d)$$

$$0 = g(x, z, u, d)$$

$$y = h(x, z, d)$$

$$J = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial z} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial z} \\ \frac{\partial h}{\partial x} & \frac{\partial h}{\partial z} \end{bmatrix}$$

after step 1

$$\frac{dx'_1}{dt} = f'_1(x', z, u, d)$$

$$0 = f'_2(x', z, u, d)$$

$$0 = g(x', z, u, d)$$

$$J = \begin{bmatrix} \frac{\partial f'_1}{\partial x'_1} & \frac{\partial f'_1}{\partial x'_2} & \frac{\partial f'_1}{\partial z} \\ \frac{\partial f'_2}{\partial x'_1} & \frac{\partial f'_2}{\partial x'_2} & \frac{\partial f'_2}{\partial z} \\ \frac{\partial g}{\partial x'_1} & \frac{\partial g}{\partial x'_2} & \frac{\partial g}{\partial z} \end{bmatrix}$$

after step 2

$$\frac{dx'_1}{dt} = f'_1(x', z, u, d)$$

$$[x'_2 \quad z] = g'(x'_1, u, d)$$

$$y = h(x', z, d)$$

$$J = \begin{bmatrix} \frac{\partial f'_1}{\partial x'_1} \end{bmatrix}$$

# POD and grey-box modeling

original model

$$\frac{dx}{dt} = f(x, z, u, d)$$

$$0 = g(x, z, u, d)$$

$$y = h(x, z, d)$$

$$J = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial z} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial z} \\ \frac{\partial h}{\partial x} & \frac{\partial h}{\partial z} \end{bmatrix}$$

reduced model

$$\frac{dx'}{dt} = Ax' + Bu$$

$$y = (Cx' + Du)^T \varphi$$

$$J = [A]$$

POD and grey-box modeling

# Open-loop validation

Following characteristics for full model and reduced models are compared:

- relative gain array (RGA)
- condition number
- simulations with input step changes that show directionality

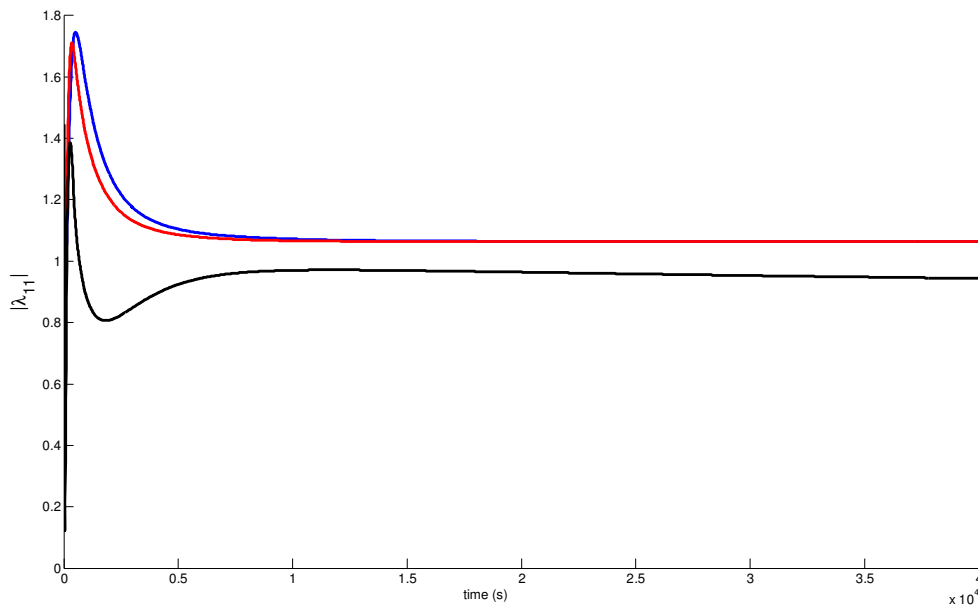
# Explanation of RGA

Numbers in RGA matrix for full model and reduced models should be the same:

$$\Lambda = \begin{matrix} & \begin{matrix} u_1 & u_2 \end{matrix} \\ \begin{bmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{bmatrix} & \begin{matrix} y_1 \\ y_2 \end{matrix} \end{matrix} \quad \text{where} \quad \lambda_{ij} = \frac{\left( \frac{\partial y_i}{\partial u_j} \right)_u}{\left( \frac{\partial y_i}{\partial u_j} \right)_y}$$
$$\sum_{i=1}^N \lambda_{ij} = 1 \quad \text{for} \quad j=1,2 \quad \sum_{i=1}^N \lambda_{ij} = 1 \quad \text{for} \quad i=1,2$$

Easy computation:  $\Lambda(s) = G(s) \otimes (G(s)^{-1})^T$  where  $s = iw$

# RGA results



blue line: full model

red line: aggregated model

black line: POD+grey-box

# Condition number

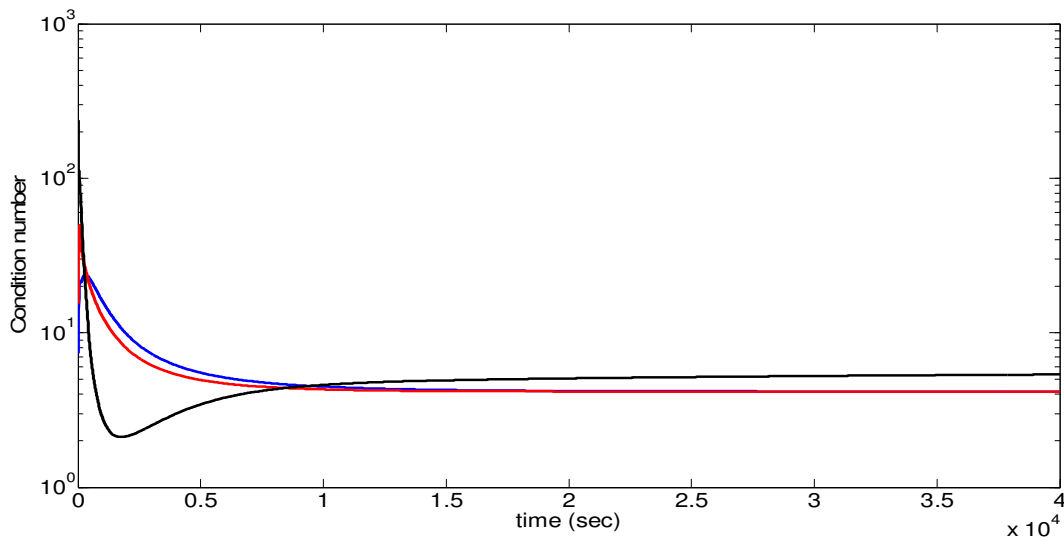
Condition number of linearized full model and linearized reduced

models should be the same:  $\gamma = \frac{\sigma_{\max}}{\sigma_{\min}}$

where  $\Sigma = \text{diag}(\sigma_1, \sigma_2, \sigma_3, \dots, \sigma_m)$  is computed by carrying out

a singular value decomposition on  $G(0)_t$ :  $G(0)_t = W\Sigma V^T$

# Condition number



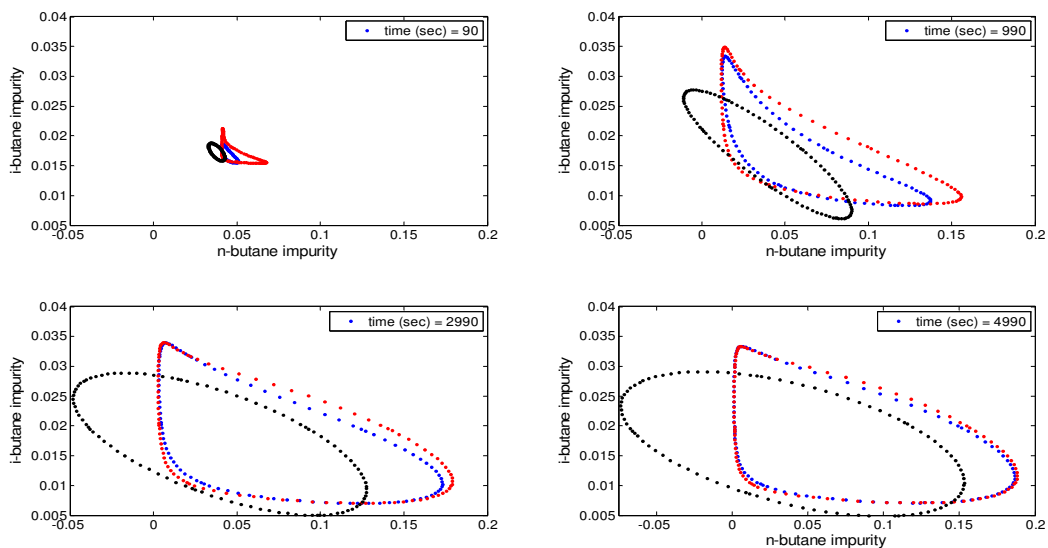
blue line: full model

red line: aggregated model

black line: POD+grey-box

# Simulations with input step changes

100 simulations with initial conditions set at at steady state values and step changes in  $u_1$  and  $u_2$  such that:  $\Delta u_1^2 + \Delta u_2^2 = 1$





## Relation simulation results $\leftrightarrow$ directionality

Axis directions of steady state output ellipses are the columns of  $W$ -matrices obtained by carrying out a singular value decomposition on  $G(0)$ :  $G(0) = W\Sigma V^T$

The  $\sigma$ -s in  $\Sigma = \text{diag}(\sigma_1, \sigma_2, \sigma_3, \dots, \sigma_m)$  determine the length of the axes.

This reasoning can be extended to non-linear systems although they do not have transfer function matrices and perfect ellipses of output values.

## Summary

- Presentation of a large DAE-model for a distillation process.
- Relation between large Jacobian of DAE-models and large computational loads.
- Presentation of two reduced models, their reduced Jacobians and reduced computational loads.
- Explanation of open-loop validation tools for reduced models: RGA, condition number, simulations with input step changes that show directionality.
- Presentation of validation results for the reduced models.