Fachgebiet dbta Dynamik und Betrieb technischer Anlagen

Optimal and Reliable Process Design and Operation by Using Chance Constrained Programming

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Outline

- Motivation
- Uncertainty problems in the process industry
- Optimization under uncertainty
- Solution approach: Chance Constrained Programming
- Application examples
- Conclusions

Optimization under Uncertainties

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Uncertain Operating Conditions:

- Future product demands, product specifications
- Future supply of raw materials, feed flow and concentration
- Availability of utilities (power, steam, …)
- Atmospheric temperature and pressure

Uncertain Model Parameters:

- Kinetic parameters
- Phase equilibrium parameters
- State-dependent parameters

Properties of Optimization under Uncertainty:

- Design (structure, sizing,…) and operation (throughput, pressure, temp.,…)
- Profit maximization / cost minimization
- Meet the operating constraints
- Consider a future time horizon (hours, days, weeks, …)
- Decision making without knowledge of exact values of uncertain variables

Handling Uncertainties in the Industry

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1. Using the Expected Value

- Base-Case-Analysis
- Too optimistic decisions (aggressive strategy)
- Violating the restrictions with a 50% probability

2. Using the Bound Values

- Worst-Case-Analysis
- Conservative strategy (no risk, safety with priority)
- Very low profit

3. Scenario Analysis

- Study more scenarios
- Relative robust decisions
- Not all cases can be considered

New Approach:
Chance Constrained Optimization

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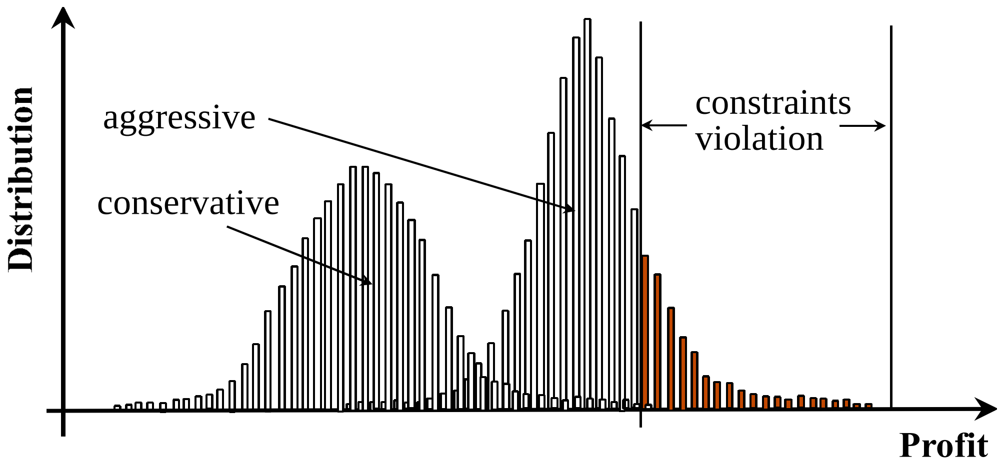
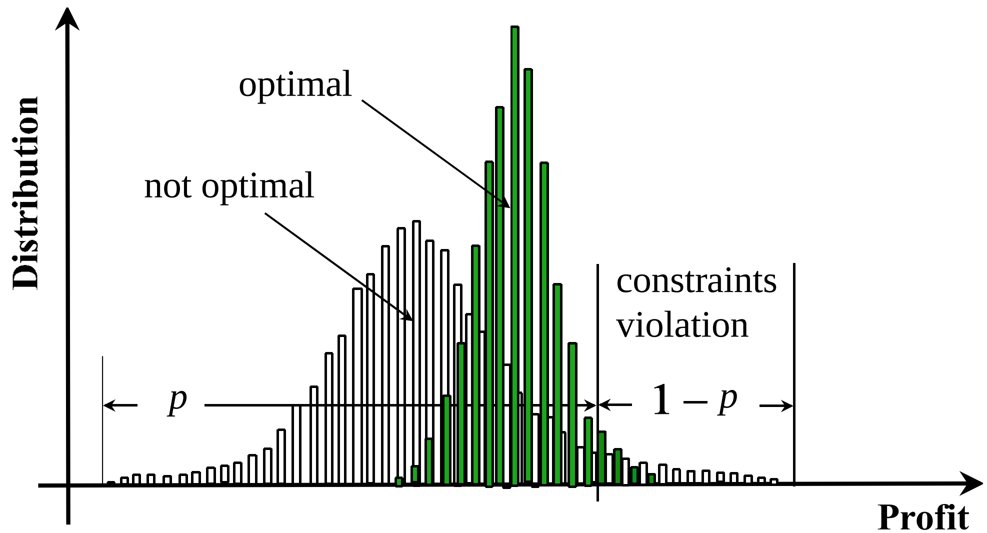
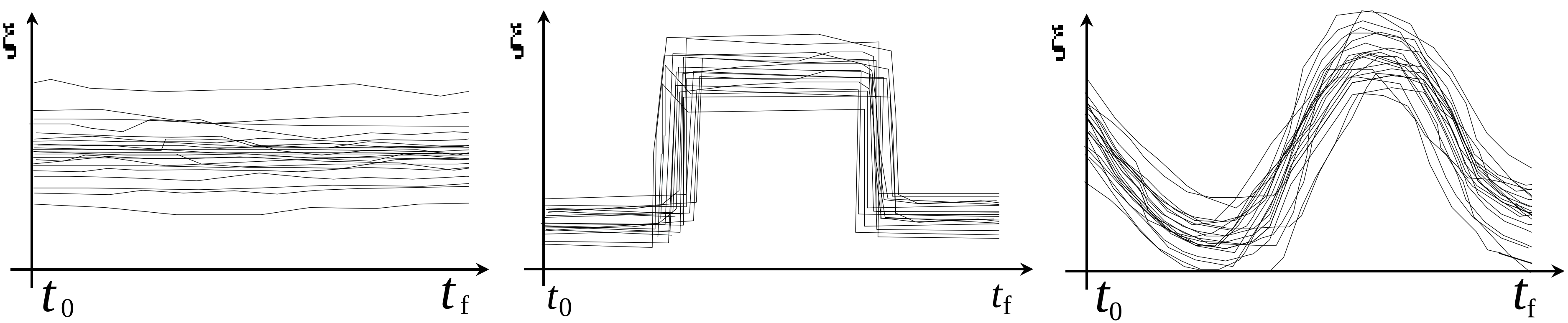
- The decision should be neither conservative nor aggressive.
- The restrictions will be satisfied with a desired probability *p* (confidence level).
- The expected value of the objective function will be optimized.
- A robust decision will be achieved (i.e. not depending on the realization of uncertain variables).





How to Describe Uncertain Variables?

- The uncertain variables behave differently.
- Their stochastic properties can be obtained based on analysis of historical data or even experiences of experts.
- Then they can be formulated according to expected values, standard deviations with probability density functions.



time-independent **stepwise** **oscillating**

Optimal Planning / Scheduling / Control under Uncertainty (linear systems)

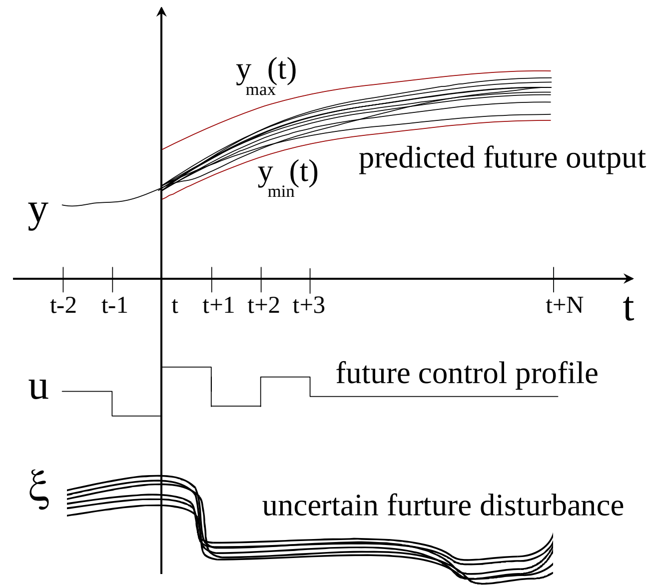
Li et al., Comp. Chem. Eng., 24(2000), 829;   Li et al., Automatica, 38(2002), 1171.

Discrete Linear Optimal Control Problem

$$\min \left[\mathbf{x}(N)^T \mathbf{S}\,\mathbf{x}(N) + \sum_{i=1}^{N-1} \mathbf{x}(i)^T \mathbf{Q}\,\mathbf{x}(i) + \sum_{i=0}^{N-1} \mathbf{u}(i)^T \mathbf{R}\,\mathbf{u}(i) \right]$$

$$\text{s.t.} \quad \mathbf{x}(i+1) = \mathbf{A}\mathbf{x}(i) + \mathbf{B}\mathbf{u}(i) + \mathbf{C}\boldsymbol{\xi}(i) \quad \mathbf{x}(0) = \mathbf{x}_0$$

$$\mathbf{y}(i) = \mathbf{F}\mathbf{x}(i), \quad \mathbf{y}_{\min} \le \mathbf{y}(i) \le \mathbf{y}_{\max}, \quad \mathbf{u}_{\min} \le \mathbf{u}(i) \le \mathbf{u}_{\max}$$



Transfer into Chance Constrained Problem

$$\min E \left[\mathbf{x}(N)^T \mathbf{S}\,\mathbf{x}(N) + \sum_{i=1}^{N-1} \mathbf{x}(i)^T \mathbf{Q}\,\mathbf{x}(i) + \sum_{i=0}^{N-1} \mathbf{u}(i)^T \mathbf{R}\,\mathbf{u}(i) \right]$$

$$\text{s.t.} \quad \mathbf{x}(i+1) = \mathbf{A}\mathbf{x}(i) + \mathbf{B}\mathbf{u}(i) + \mathbf{C}\boldsymbol{\xi}(i) \quad \mathbf{x}(0) = \mathbf{x}_0$$

$$\Pr\{\mathbf{y}_{\min} \le \mathbf{y}(i) \le \mathbf{y}_{\max}, \; i = 1, \cdots, N\} \ge p$$

$$\mathbf{u}_{\min} \le \mathbf{u}(i) \le \mathbf{u}_{\max}$$

Relax into Nonlinear Programming Problem

$$\min \; \varphi(\mathbf{u})$$

$$\text{s.t.} \quad \boldsymbol{\psi}(\mathbf{u}) \ge \mathbf{0},$$

$$\mathbf{u}_{\min} \le \mathbf{u} \le \mathbf{u}_{\max}$$

The probability and gradients of the multivariate normal distribution is computed by the inclusion-exclusion method combined with an efficient sampling approach.

Chance Constrained Nonlinear Optimization

Wendt et al., Ind. Eng. Chem. Res., 41(2002), 3621.

Nonlinear optimization problem

$$\begin{aligned}
\min \quad & f(\mathbf{x},\mathbf{u},\xi) \\
\text{s.t.} \quad & \mathbf{g}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi)=\mathbf{0}, \quad \mathbf{x}(t_0)=\mathbf{x}_0 \\
& \mathbf{y}=\mathbf{h}(\mathbf{x},\mathbf{u},\xi) \\
& \mathbf{y}_{\min} \le \mathbf{y} \le \mathbf{y}_{\max} \\
& \mathbf{u}_{\min} \le \mathbf{u} \le \mathbf{u}_{\max} \\
& t_0 \le t \le t_f
\end{aligned}$$

The chance constrained problem

$$\min \; E\left[f(\mathbf{x},\mathbf{u},\xi)\right] + \omega\, D\left[f(\mathbf{x},\mathbf{u},\xi)\right]$$

s.t.

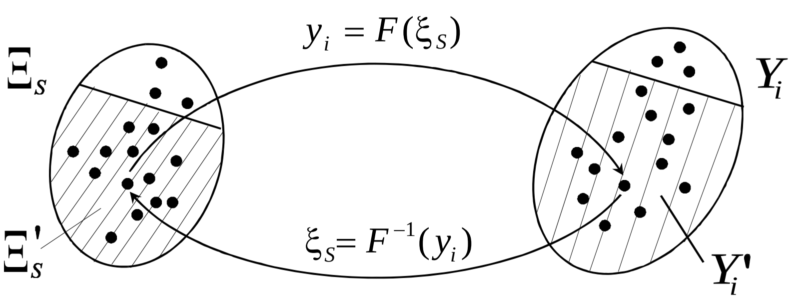
$$\Pr\left\{y_i^{\min} \le y_i(\mathbf{u},\xi) \le y_i^{\max},\ i=1,\cdots,I\right\} \ge p$$

or

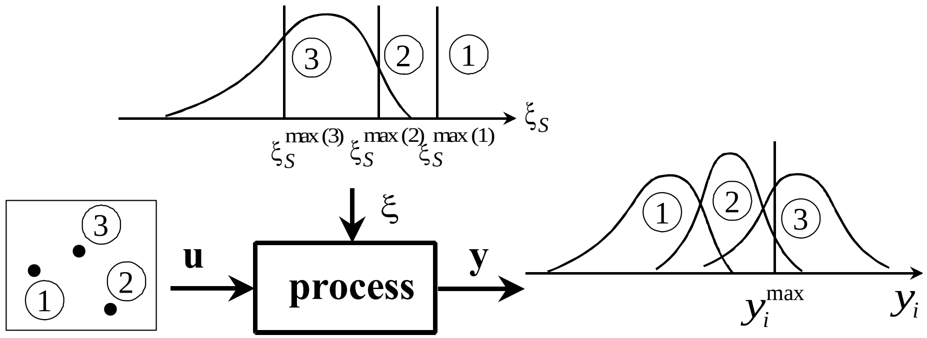
$$\Pr\left\{y_i^{\min} \le y_i(\mathbf{u},\xi) \le y_i^{\max}\right\} \ge p_i,\quad i=1,\cdots,I$$

$$\mathbf{u}_{\min} \le \mathbf{u} \le \mathbf{u}_{\max}$$

Back mapping from output to input

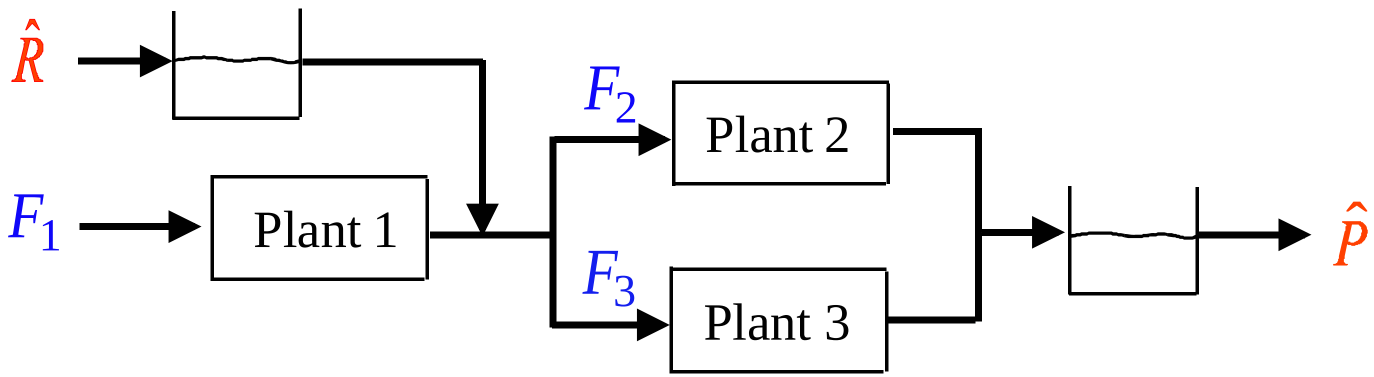


The probability computation scheme



Example 1: Optimal Production Planning of a Multi-plant Process

Profit maximization under uncertain Supply and product demand



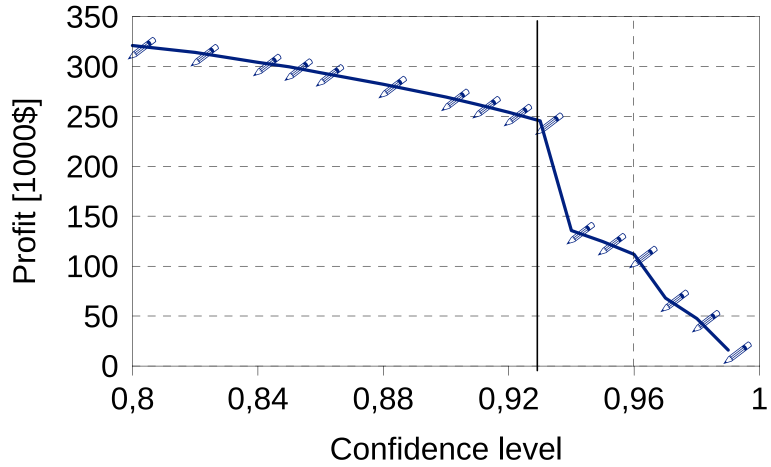
Problem definition:

- Planning the production strategy for the next 5 time period.
- There is the possibility to switch over the plants (structure changes).
- Expected values and variances of the uncertain variables are given.
- Expected price factors are known.

Example 1: The Optimization Results

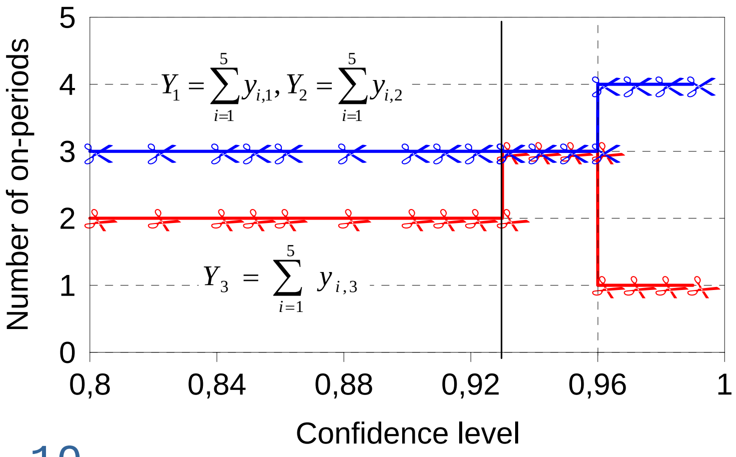
Li et al., Chem. Eng. Tech., 27 (2004), 641.

Profit versus Reliability

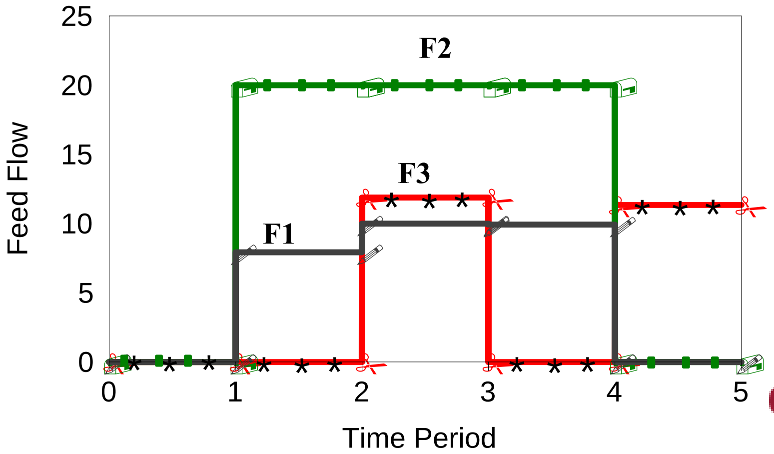


- If p makes a structure change necessary, then there will be a stepwise decrease of the profit.
- This point is suitable for determining optimal decisions for the Production.

On-Periods of the Plants



Optimal operation strategy at $p = 0{,}93$



Example 2: Optimization of Operation Policies for a Reactive Semi-batch Distillation process

Chemical Reaction:

$$\underset{(A)}{\text{educt ester}} + \underset{(B)}{\text{educt alcohol}} \underset{k_R}{\overset{k_H}{\rightleftharpoons}} \underset{(C)}{\text{product ester}} + \underset{(D)}{\text{product alcohol}}$$

Aim of the Optimization:

Minimization of the batch time

Uncertain Variables:

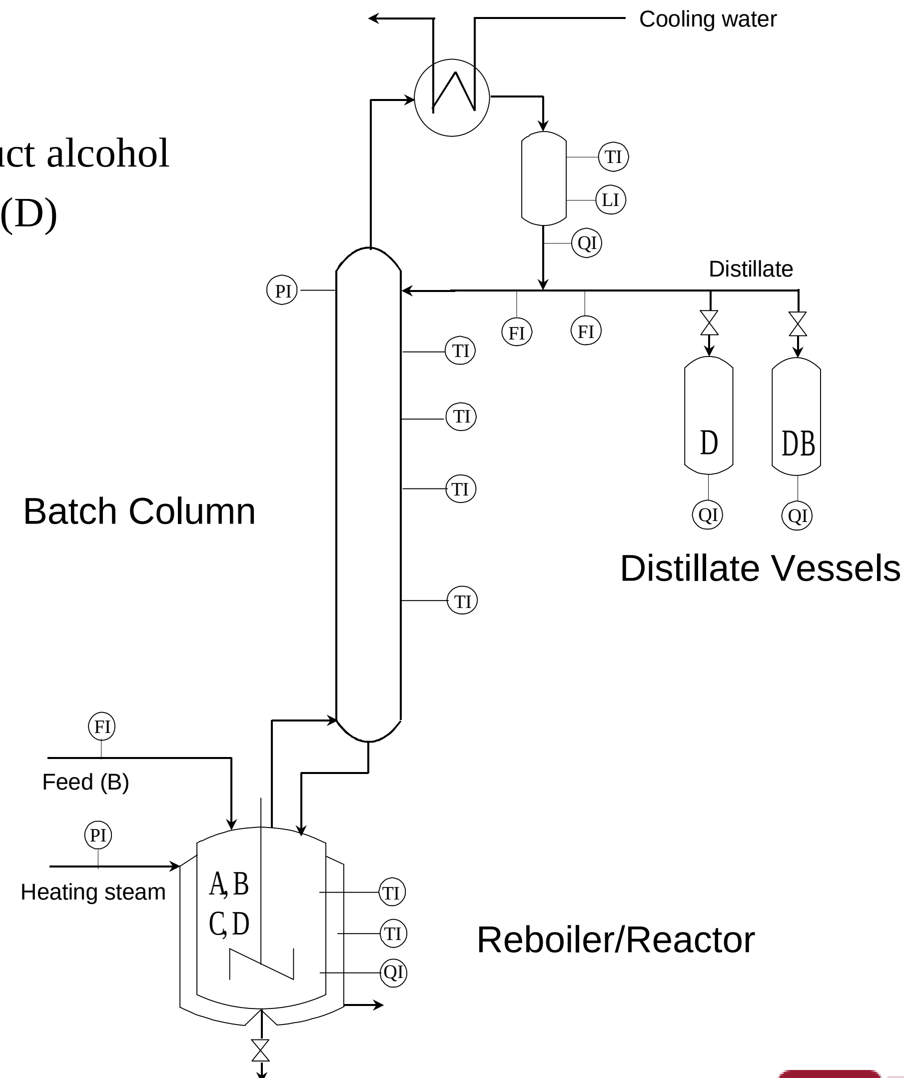
- Kinetic parameters
- Tray efficiency
- Initial charge

Product Specifications:

- Product alcohol concentration ≥ 98%
- Educt ester concentration ≤ 2%

Optimization Variables:

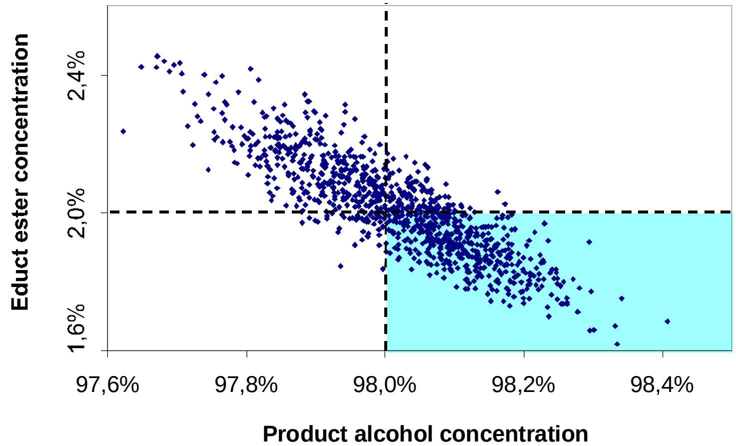
- Reflux flow rate policy
- Educt alcohol dosage policy



Example 2: The Optimization Results

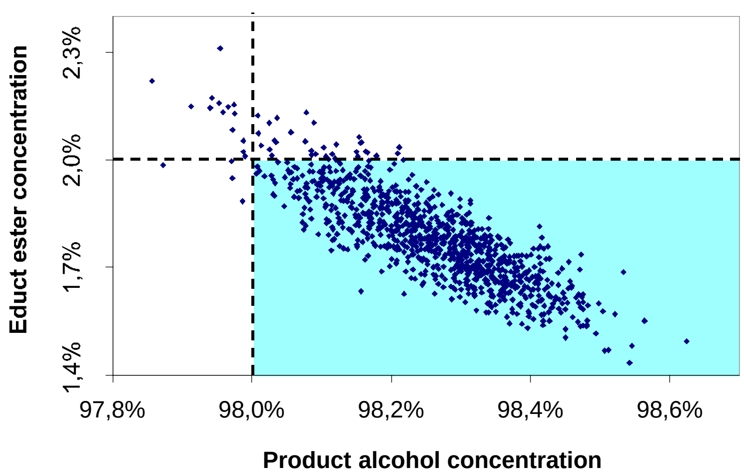
Arellano et al., Chemie-Ingenieur-Technik, 75 (2003), 822.

Product concentration based on deterministic Optimization



By realizing the deterministic optimal policy there will be a 50% probability to violate the product specifications.

Product concentration based on stochastic Optimization



By realizing the stochastic optimal policy there will be only 4% probability (as desired) to violate the product specifications.

Example 3: Application to a Process Design Optimization Problem

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Challenges:

- Distributions of uncertain variables are unknown.
- The uncertain variables are described in intervals.
- A 100% reliability must be guaranteed.
- Design has to be feasible as well as optimal.
- The feasible region is to be identified for design.

For example:

$$g_1 = 0.08u^2 - \theta_1 - \frac{1}{20}\theta_2 + \frac{1}{5}d_1 - 13 \le 0$$

$$g_2 = -u - \frac{1}{3}\theta_1^{1/2} + \frac{1}{20}d_2 + \frac{1}{5}d_1 + 11\frac{1}{3} \le 0$$

$$g_3 = \exp(0.21u) + \theta_1 + \frac{1}{20}\theta_2 - \frac{1}{5}d_1 - \frac{1}{20}d_2 - 11 \le 0$$

- **Design Variables:** d_1, d_2
- **Uncertain Variables:**

  $2 \le \theta_1 \le 4,\ 2 \le \theta_2 \le 4$
- **Control Variable:** u

What is the feasible region for design?

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Example 3: The Optimization Results

Li et al., FOCAPD, Princeton, 2004, Proceedings pp. 514-518.

Probability maximization problem

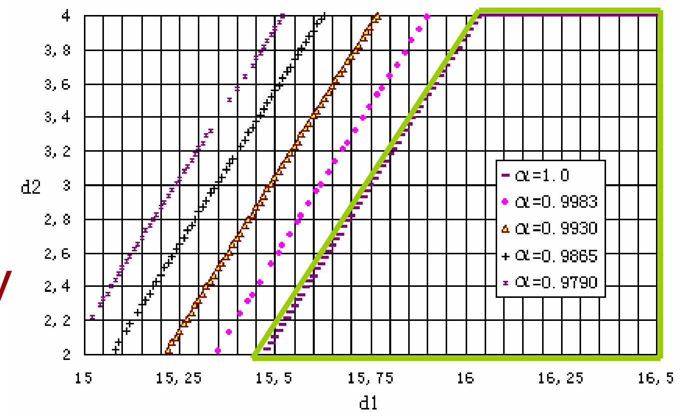
$$\max_{\mathbf{u},\alpha} \ \alpha$$

$$\text{s.t.} \quad \Pr\left\{ g_l(\mathbf{u},\boldsymbol{\theta},\hat{\mathbf{d}}) \le 0 \right\} \ge \alpha, \quad l = 1,\cdots,L$$

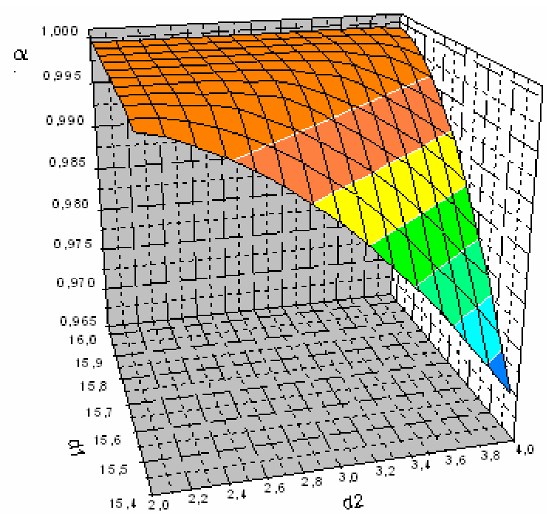
$$\mathbf{u}_{\min} \le \mathbf{u} \le \mathbf{u}_{\max}$$

Feature: Feasible region over 100% reliability is not dependent on distributions!

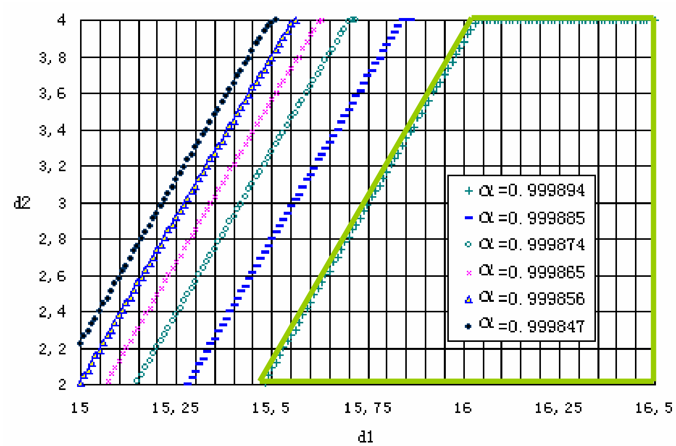
Feasible region under uniform distribution



Reliability levels vs. different design



Feasible region under normal distribution



Conclusions

- The process industry nowadays uses deterministic optimization approaches.
- Off-line, on-line process optimization is being carried out.
- Challenging task: Solution of large-scale, complex optimization problems under various uncertainties.

New Solution Approach:

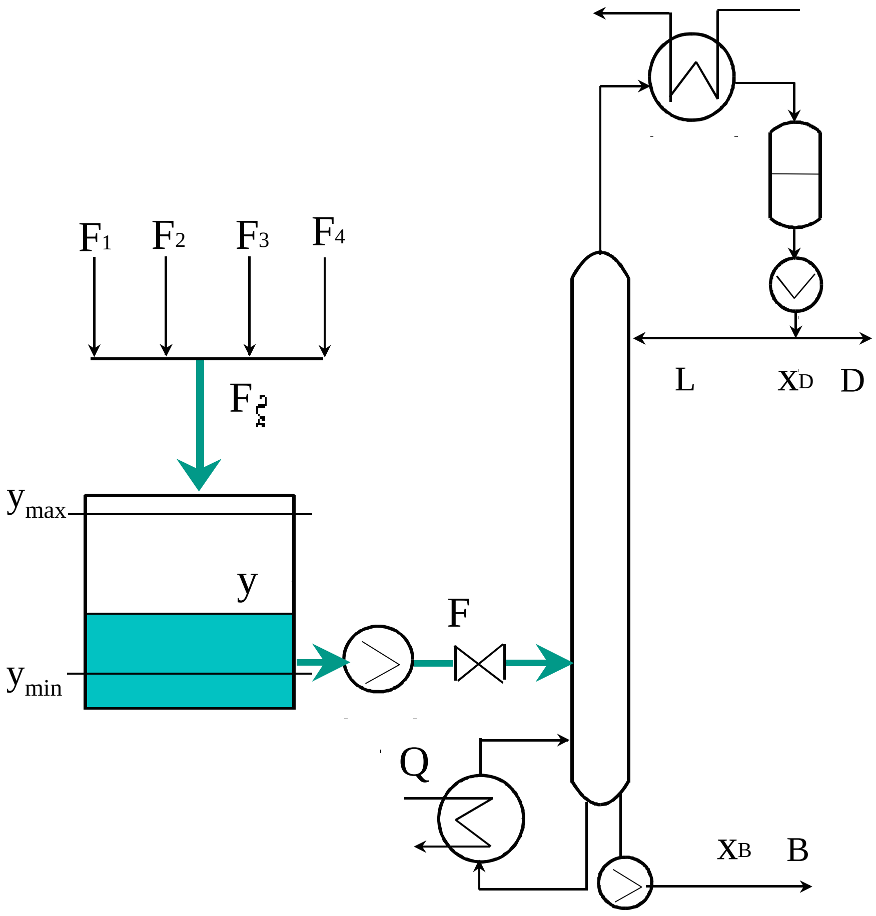
- General concept to consider uncertain operating conditions as well as uncertain model parameters.
- Solve the problem with stochastic programming under chance constraints.
- Application to different optimization tasks in the process industry.
- The solution provides optimal as well as reliable decisions.

Future work:

- Application to large-scale problems
- On-line optimization under uncertainty

Example 4: Optimal Operation of a Distillation Column under Uncertain Feed flow

Li et al., AIChE Journal, 48(2002), 1198.



A common problem:

- Feed flow is from upstream plants
- Different stochastic distributions.
- Total flow is small in the night and at weekends.
- It is large on normal working days.

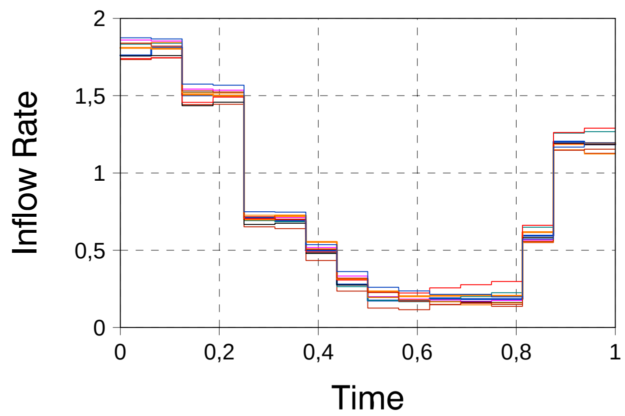
Consequences:

- Tank level higher than upper bounds: Special Vessels are needed.
- Tank level lower than lower bound: The column has to be operated with recycle.
- Column operating point will be significantly disturbed.

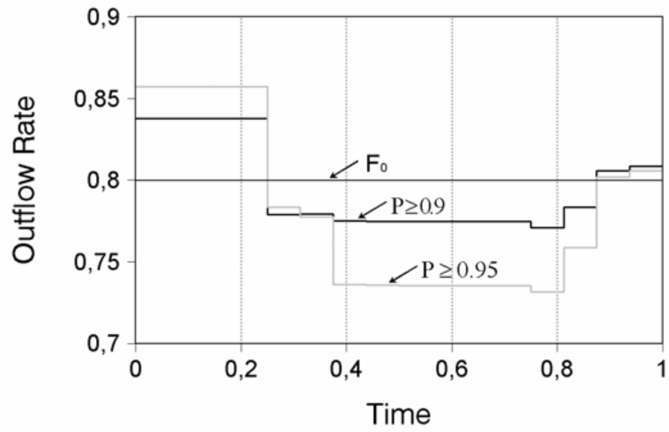
Example 4: The Optimization Results

Aim of Optimization: Minimization of the oscillations of the feed flow to the column under the tank capacity

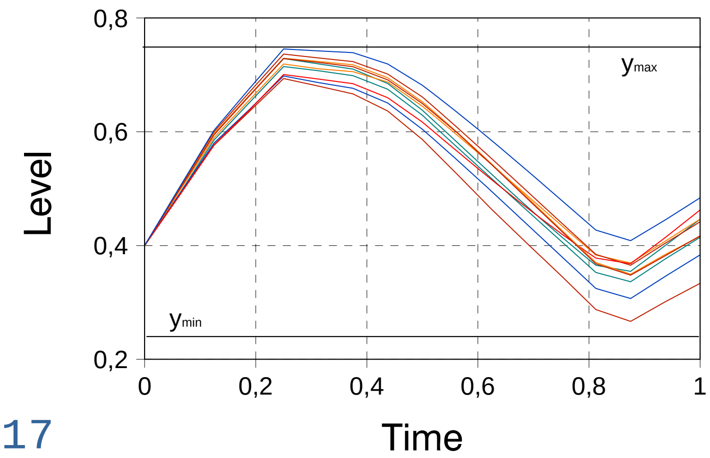
10 samples of the total feed flow



Optimal feed strategy to the column



Tank level by 10 disturbances ($p \geq 0.95$)



Tank level by 10 disturbances ($p \geq 0.9$)