

ROBUST ONLINE OPTIMIZATION BASED ON CONTROLLER PERFORMANCE METRICS FOR A HIGH-PRESSURE DISTILLATION COLUMN

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In the daily production of chemical industry numerous plant and units are operated to satisfy product requirements. Following the optimal operation planning, predefined steady state operating points for continuous processes are assigned to a process control system. However, a closed-loop control involves online measured values of controlled variables. Consequently, the non-measurable variables are then open-loop even though they have to be constrained. Yet to guarantee the product quality, particularly conservative set-point values are selected in industrial practice which inevitably leads to unnecessary high costs. In this work, we propose a chance-constrained optimization approach in which the objective function will be improved while satisfying constraints to enforce product quality restrictions with a desired probability (confidence) level. This result in a new concept of control: to control open-loop processes by closed-loop control. Unlike the definition where controls are decision variables, in the proposed closed framework the set-points of the measurable outputs are defined as decision variables. Moreover, the controller performance based on the minimum variance control can be regarded as a random input, and thus is also included in the chance-constrained formulation of the model-based stochastic optimization problem. Consequently, the result is a cyclic adjustment of the operating point which guarantees the compliance with the product quality restrictions and assures the controller performance under parametric uncertainty, uncertain boundary conditions, and the random regulatory deviation. To demonstrate its efficiency, the approach is applied to the optimal operation and control of one column embedded in a coupled two-pressure column system for the separation of an azeotropic mixture.

KEYWORDS: online optimization, uncertainty, robustness, controller performance, chance constrained programming, two-pressure column system, azeotropic mixture

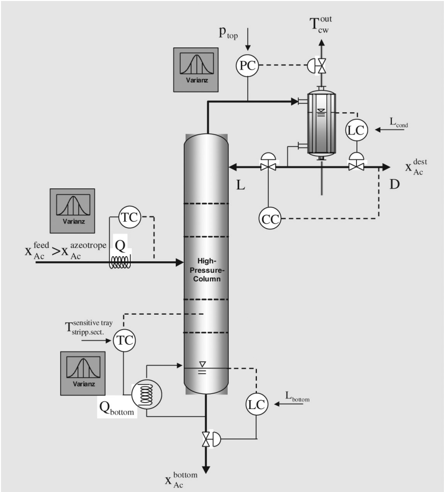
INTRODUCTION

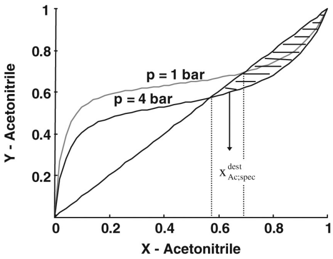
Process industries in today's highly competitive market and needs for product quality must reconsider their production control policies and strategies if they are to achieve sustainable production and increase their competitiveness. Therefore, it is necessary to take a holistic view of process management. This can only be accomplished by integrating product quality and process economy impact in process control and optimization system. Thus, there have been a lot of efforts in optimizing existing plants and using their full application potential. The generation and implementation of optimal control strategies can be achieved through a hierarchical system of layers. In the optimization upper layer decisions about the optimal process state with respect to various objectives are made. The results are then sent in form of set-points to the regulatory control layer where the optimal strategies are implemented keeping the system state at the optimal operating point. However, the inherent plant disturbance spectrum leads inevitably to controller performance deviations from their optimal set-points. This causes a significant detrimental effect on plant profitability. Moreover, if the optimal operating point lies on active constraints, violation of process limitations seems to be unavoidable. Overstepping the constraints makes the operation infeasible, which not only means a loss of quality but also a safety risk. Accordingly, the challenge of plant operation optimization lies in reducing the conservative distance to the constraints and pushing the plant to its limits without exceeding critical limitations. To guarantee robust implementation of optimal decisions, the controller deviations and uncertainties are required to be part of the control structure i.e. to integrate implementation errors and stochastic parameters in the process model. By this means, effects of disturbances and model uncertainties can be compensated and robust set-points for the regulatory control layer are then obtained.

PROBLEM STATEMENT

A high-pressure column embedded in a coupled two-pressure column system for the separation of an azeotropic mixture (Acetonitril-Water) is considered to demonstrate the efficiency of the proposed approach which is applied to guarantee an optimal robust operation and control. Due to the operational characteristics of the pressure swing system the consideration of the individual high-pressure column does not imply a loss of general validity with regard to the operability of the whole system. The operating point is defined by the distillate and bottom product specifications, cooling outlet temperature limitations, as well as the maximum pressure of the considered high-pressure column. Figure 1 shows the individual high-pressure column and the control loops corresponding to the regulatory control layer. A binary homoazeotropic mixture consisting of acetonitril/water is fed into the column. Here, the feed has a higher acetonitril concentration than the azeotropic point. The increase of the operating pressure causes a movement of the distillation boundaries in the composition space. Operating the illustrated high-pressure column above the azeotropic point results in pure *acetonitril* as bottom product. The complete separation task is carried out by means of pressure swing distillation. By this means, the distillate of the high-pressure column is fed to the low-pressure column where water is obtained from the bottom.

Using a validated rigorous model based on physical and thermodynamics principles, nominal optimal decisions are determined by solving an optimization problem. The objective function is defined as the minimization of the total energy required subject to product quality as well as safety related constraints. This yields a large-scale NLP problem which is solved via SQP following the sequential strategy. The deterministic optimization





Column set-up: 28 trays, diameter 0.1m, Feed acetonitrile/water, 25 l/h, 76 mole%	
Constraints:	Deviations / Uncertainties
$x_{Ac;spec}^{dest} = 62.5$ mole%	$\sigma(p_{top}) = 0.04$bar
$x_{Ac;spec}^{bottom} = 99.5$mole%	$\sigma(T_{sens}^{stripp}) = 0.65$K
$p^{max} = 4$bar	$\sigma(x_{Ac}^{feed}) = 4$mole%
$T_{cw}^{max} = 70°C$	

Figure 1. *Left*: Regulatory control layer of the high pressure column; *top right*: VLE diagram acetonitril/water; *down right*: operational conditions

problem can be formulated as follows,

$$\begin{array}{cl}
\min\limits_{Q_{bottom},r,m_{cw},L_{cond}} & \dot{Q}_{bottom} \\
\text{s.t.} & \text{model equations} \\
 & \left.\begin{array}{ll} x_{Ac}^{dest} & \leq x_{Ac;spec}^{dest} \\ x_{Ac}^{bottom} & \geq x_{Ac;spec}^{bottom} \end{array}\right\}\text{product quality restrictions} \\
 & \left.\begin{array}{ll} p_{top} & \leq p^{max} \\ T_{cw}^{out} & \leq T_{cw}^{max} \end{array}\right\}\text{safety restrictions}
\end{array} \tag{1}$$

Where $x_{Ac;spec}^{dest}$ and bottom $x_{Ac;spec}^{bottom}$ are the product purity specifications concerning the high-pressure column, p^{max} and T_{cw}^{max} are the maximal allowable system pressure and cooling outlet temperature, respectively. The decision variables are the reboiler duty $\dot{Q}_{bottom}$, the reflux rate, the cooling flow rate $\dot{m}_{cw}$ as well as the level in the condenser L_{cond}. The system pressure is kept at its operating value by adjusting the energy balance in the condenser i.e. varying the heat transfer through manipulation of the condenser level L_{cond} and the cooling flow rate. The heat flux in the overhead condenser is carried out through variation of cooling water temperature and effective surface area. The operating range is though limited by the product specifications and the maximal system pressure as well as the cooling outlet temperature. Thus, at the nominal optimal solution all constraints are active. This means that an energy-optimal operation is defined by means of covering the minimal requirements for product quality and driving the plant at its upper safety limits. For this specific problem, the column efficiency of the right side of the azeotropic point is favored with increasing pressure, decreasing the relative volatility (here the relative volatility is minor than one). Also the system pressure reduces the vaporization heat. For the specific separation problem discussed here, the higher the pressure the more is the azeotropic point shifted towards lower concentrations of acetonitril supporting the separation in the rectifying section of the column. High pressure is crucial for the formulated separation problem and leads to less energy requirements. Furthermore, in order to keep the cooling water temperature at its maximum value and the condenser level L_{cond} small, the temperature of the reflux is then also maximal. However, from the energetic point of view this effect plays a minor role.

ROBUST OPERATION OF THE HIGH-PRESSURE COLUMN

As stated before, operation with a minimal amount of energy is determined by the boundary conditions of the quality specifications and the maximal allowable pressure. However, operating the plant at these boundaries results inevitably in constraint violations. The presence of disturbances, parametric uncertainties and implementation errors may provoke infeasibility and a quality loss.

To overcome these problems, one straightforward way is to introduce a back-off from the nominal optimum in order to avoid infeasibility. However, the key idea is here to define the optimal operational range in the optimization layer and to send the results as set-points to the regulatory control layer. The basis controllers will stabilize the plant continuously and closed-loop variances will then be determined and sent back to the upper layer (Figure 2 left). By using this information in the optimization layer, implementation errors and model uncertainties are determined in order to compute the optimal and

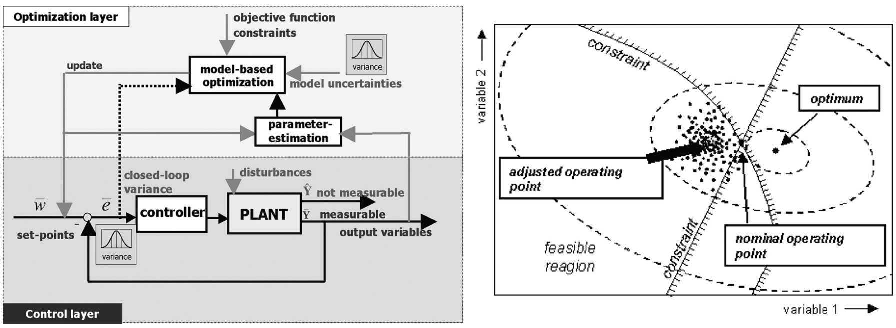


Figure 2. *Left*: Two-layer control for robust operation; *right*: constrained optimization problem and back-off for robust operation

robust set-points. Thus, a cyclic adjustment of the set-points guarantees feasible and optimal operation in the presence of changing plant conditions. The difference between nominal and adjusted operating point is here called back-off. To illustrate the principle of adjusting nominal decisions, Figure 2 right shows exemplarily a constrained optimization problem of two independent process states. At the nominal result two constraints are active and the state variables are to be kept at their operating point by the regulatory control layer. To account for the dynamic region around the nominal optimum, the set-points have to be adjusted. The dimension of the dynamic region can be obtained by controller quality metrics, like the closed loop variance. It only depends on the controller performance as a function of the plant disturbance spectrum at the current steady state. In order to operate as close as possible at the optimum, the back-off has to be minimized while still satisfying all constraints.

ACCOUNTING FOR UNCERTAINTIES AND CONTROLLER VARIANCE

In the presence of variations of state variables, robust and optimal decisions can be obtained accounting for these stated deviations. Deviations from set-point are also called implementation error d_c (Govatsmark, 2005) and in the following assumed to be known by measuring the closed loop variance of the state variable. Usually constrained variables are measured and controlled directly, in particular, if the respective constraints are safety related. At the operation stage, processes are usually run with an operating point defined by worst case estimation of the variability. For the example discussed here, the constraints corresponding to the maximum allowable system pressure and the cooling water outlet temperature are transient constraints which have to be satisfied at any time. The constraints can simply be adjusted by tightening the maximal value.

$$x^{max} = x^{max}_{nominal} - d_c \tag{2}$$

The product specifications are considered to be steady constraints. They may be violated during transients but not at steady state or in average. Besides, the concentration in the stripping section is controlled by keeping the temperature constant on the sensitive tray. Thus, the implementation error concerns the temperature since the product specifications can not be adjusted directly. Perkins and co-workers show for linear model predictive control how to determine the co-variances of constrained input and output variables and use this information to find out the required back-off from process limitations. This approach assumes a linear system where the constraints are hold with a defined probability. However, methods of solving chance-constrained optimization problems for nonlinear processes under uncertainty is a challenging task. The main challenge lies in the difficulty in determining the probability of the output constraints and its sensitivity. Furthermore, in most of the practical relevant applications, the relation between measured variable and constrained variable depends on nonlinear physical relations expressed by the model equations. To account for the measured closed loop variance of the temperature and pressure, respectively, uncertainties have to be explicitly taken into consideration in the

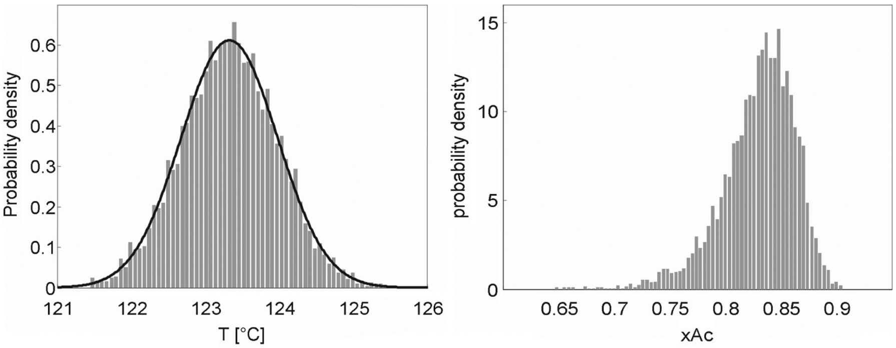


Figure 3. *Left*: Gaussian probability distribution of the temperature; *right*: effect on the concentration of acetonitril using VLE (p = 3.85 bar)

model equations. Like other disturbances or model uncertainties, they can be expressed as uncertain parameters. In the following sections, the feed concentration is assumed to be stochastic Gaussian noise defined by mean and standard deviation. To demonstrate the influence of stochastic parameters on the model equations, Figure 3 shows the probability density functions of temperature and concentration of acetonitril, respectively. For this purpose, a simple VLE model is used with constant pressure and Gaussian noise is added to the known temperature. Solving the equations many times by stochastic sampling (Monte-Carlo-simulation), the spectrum of the concentration is obtained as the output deviation. It can be seen that the nonlinear relationship between both variables affects also the distribution of the uncertain constrained output variable.

OPTIMIZATION UNDER UNCERTAINTY – THE SOLUTION APPROACH

Generally, a nonlinear optimization problem under uncertainty can be formulated as follows:

$$\begin{aligned} \min \quad & f(\mathbf{x}, \mathbf{u}, \boldsymbol{\xi}) \\ s.t. \quad & \mathbf{g}(\mathbf{x}, \mathbf{u}, \boldsymbol{\xi}) = 0 \\ & \mathbf{h}(\mathbf{x}, \mathbf{u}, \boldsymbol{\xi}) \leq 0 \\ & \mathbf{x} \in X, \mathbf{u} \in U, \xi \in \Xi \end{aligned} \tag{3}$$

where f is the objective function, g and h are the vectors of the equality and inequality constraints, while $\mathbf{x} \subseteq \Re^n$, $\mathbf{u} \subseteq \Re^m$ and $\boldsymbol{\xi} \subseteq \Re^S$ are the vectors of state, decision and uncertain variables, respectively. One way of handling the uncertainties is to transform the inequality constraints to chance constraints with a user predefined probability level. However, in nonlinear systems, the type of the probability density function (PDF) of the uncertain input is not the same as the one of the constrained output. Unlike linear systems, a multivariate normal distribution of the input never causes a multivariate normal distribution of the output. The PDF of the output is mostly not even known. Thus a transformation performed for linear systems is not possible. The chance constraints can be either computed through efficient sampling techniques or numerical integration techniques. The latter one has been accomplished (Arellano-Garcia et al. 2003) in the case of a monotone relation between the constrained output and at least one uncertain input. This method is applicable to all stochastic optimization problems where uncertainty can be described by any kind of joint correlated multivariate distribution function. In this method, an equivalent representation of the probability is derived by mapping the output feasible region to a integration region of the uncertain inputs. This implies that the probability of holding the output constraint can be computed by integration in the corresponding region of the uncertain variable. It should be noted that all uncertain variables, which have an impact on the constrained output variables, are taken into account when computing the probability. In addition, the values of the decision variables have also an impact on the projected region. Furthermore, in order to link this method to a NLP framework, the gradient computation of the output constraint probability to the decision variables is required (Arellano-Garcia et al., 2004). In this work, for the numerical integration collocation on finite elements is used.

To solve the optimization problem under uncertainty, special treatments to the objective function, the equality and inequality constraints have to be made in order to relax the stochastic optimization problem to an equivalent NLP problem and solve it with an standard NLP solver such as SQP. For the evaluation of the objective function, the inequality constraints and their sensitivities to the decision variables, a multivariate integration is required. For instance, if $y(\mathbf{u}, \boldsymbol{\xi})$ represents a constrained output variable e.g. the product concentration in the bottom, it can be seen that due to the uncertainties $\boldsymbol{\xi}$, it is impossible to hold its limitations for sure. Hence, since the constraint is affected by the uncertain parameters, it should be reformulated to chance constraints. Consequently, a probability level will be defined to represent the reliability of being feasible. This leads to the formulation of a single chance constraint:

$$\Pr\{y(\mathbf{u}, \boldsymbol{\xi} \leq y^{spec}\} \geq \alpha \tag{4}$$

where Pr represents the probability measure and α the probability level defined by the process operation requirements. Since the uncertain parameters also have an impact on the objective function, the usual way is to reformulate it to its expected value. However, for practical application, it is more convenient to assure a certain reliability of the realization of the calculated objective value. This can be achieved by minimizing an upper bound β, which is independent of the uncertain parameter space Ξ, and the compliance of it can be guaranteed with a certain reliability by formulating an additional chance constraint (Arellano-Garcia et al., 2004). Besides, minimizing β means, in this case, to tighten the respective constraint and the feasible optimization region (see Equation 5).

FORMULATION OF THE NONLINEAR CHANCE CONSTRAINED OPTIMIZATION PROBLEM

In the following section, the formulation of the nonlinear chance-constrained optimization problem is presented. As described above, the system possesses 4 degrees of freedom. The condenser level and the cooling water rate keep the pressure at the maximum defined by the safety constraints. However, the problem is reformulated and, thus, two important modifications are considered in comparison to the deterministic formulation. First, in order to reduce the computational effort, pressure and cooling outlet temperature are set constant with the necessary back-off from the nominal optimum so as to satisfy the safety constraints (see Equation 2). By this means, the level and the cooling water rate are computed by solving the model equations. Second, the decision variable, reboiler duty Q_{reb}, is substituted by the temperature of the sensitive tray in the stripping section. In this way, the implementation error of the temperature control in the stripping section can be expressed including only one stochastic parameter in the energy balance of the corresponding tray. We define $\bar{\xi}$ as the stochastic parameters which express the implementation error of the pressure and temperature control loop. Furthermore, deviations in the feed concentration are treated as uncertainty or external disturbances. Finally, deviations in the cooling water outlet temperature are neglected due to the minor effect on the energy balances in the column. As discussed in the section above, the objective function is replaced and an additional single chance constraint is formulated with respect to the original objective function and included in the optimization problem. This leads to the following formulation of the optimization problem,

$$
\begin{aligned}
\min \quad & \beta \\
\text{s.t.} \quad & \text{model equations,} \\
& \text{direct adjusted state variables:} \\
& T_{CW}^{out} = T_{CW,ref}^{out} + b_T[\sigma(T_{CW}^{out})], \\
& P_{top} = P_{top,ref} + b_P[\sigma(P_{top})], \\
& \text{indirect adjusted constrained output variables:} \\
& \Pr\{x_{Ac}^{B} \geq x_{Ac,spec}^{B}\} \geq \alpha_1, \\
& \Pr\{x_{Ac}^{D} \leq x_{Ac,spec}^{D}\} \geq \alpha_2, \\
& \text{originally replaced objective function as chance constraint} \\
& \Pr\{\dot{Q}_B \leq \beta\} \geq \alpha_3, \\
& \text{Uncertainties and probability levels:} \\
& \bar{\xi} = [\sigma(P_{top}); \sigma(T_{strip}^{sens}); \sigma(x_{Feed});], \ \alpha = [95\%; 95\%; 90\%] \\
& \text{and finally regulatory deviation variance.}
\end{aligned}
\qquad (5)
$$

The resulting nonlinear chance constrained optimization problem is relaxed to an equivalent NLP problem and can then be solved using the SQP algorithm. The solution of the optimization aims to minimize the necessary back-offs holding the product specifications with the predefined probability levels.

NUMERICAL RESULTS

Feasible operation is obtained by explicit inclusion of closed-loop deviations and model uncertainty in the problem formulation. This is realized in two different ways: forcing a direct or and indirect back-off from the nominal optimal solution (see Equation 5). To consider additional implementation errors and model uncertainties in the model equations, the optimization problem can be reformulated. By this means, changing independent and state variables (see closed-loop deviation of the temperature in the stripping section). However, the result of the optimization problem are robust variables which are then sent to the regulatory control layer defining the set-points. To assure feasible and optimal operation under changing implementation errors and uncertainties a cyclic adjustment of the set-points is proposed. Figure 4 shows the results of the robust optimization. It should be noted that closed loop variance of the pressure, the temperature control on the 5th tray of the stripping section, as well as the uncertain feed concentrations are considered. By application of the Monte Carlo sampling method, the distribution of all variables for the known model uncertainties and deviations in the closed-loops can be simulated. Deviations around the robust operation point in the temperature profile over the column and the product concentrations are also shown in Figure 4.

Table 1 shows the optimal results w.r.t. a minimal reboiler duty. In comparison with a conventional operating point with product concentrations wide beyond the product specifications, the robust operation strategy is close to the nominal optimum satisfying the safety criterions and keeping the specifications with a probability of 95%.

CONCLUSIONS AND OUTLOOK

An approach to robust and optimal operation of a high-pressure column has been presented. In order to satisfy the operational constraints the nominal optimal decisions are adjusted cyclical. Thus, in this work, a two-layer approach for integrating model based online optimization and control is presented. Fast disturbances are treated in the basic regulatory control layer whereas in the optimization layer optimal set-points are computed.

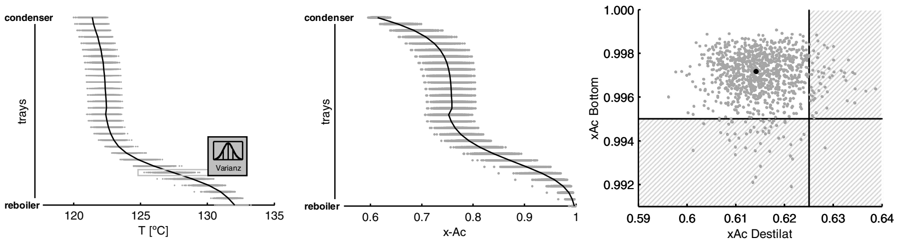


Figure 4. *Left/middle*: robust temperature/concentration profile and deviations, controlled temperature on the 5th tray; *right*: distribution of the product concentrations around the robust optimization result

Table 1. Optimization results for nominal, robust and conventional operation

	Operating point		
	Nominal	Robust	Conventional
x_{Ac}^{Dest}	0,625	0,614	0,58
x_{Ac}^{Bottom}	0,995	0,997	0,9999
$\dot{Q}_{Reb}$	4,53 KW	4,87 KW	6,79 KW

Explicit inclusion of closed-loop deviations and model uncertainty in the problem formulation guarantee feasible and optimal operation. The application of the developed methodology will be presented by implementation of a soft-sensor in order to compute optimal set-points for the temperature control loop. Furthermore, solving a reduced model for the stripping section, robust set-points are evaluated to meet the bottom product specification.

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