# Dynamic Optimization of an Evaporator with a Nonlinear Model Predictive Controller for Application at Modular Micro Rectification

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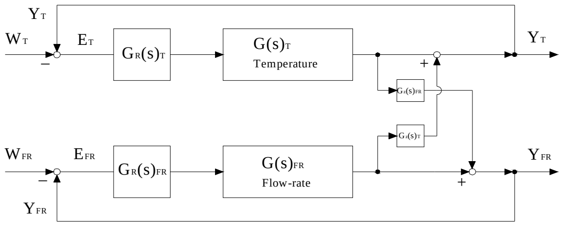
Intensification and Optimization of unit operation distillation and thus in further consequence of rectification process should be carried out as main objective of this work. A combination of Micro Process Engineering and Advanced Process Control (APC) is therefore applied to latter separation process.

Vapour and liquid phases of a simple batch distillation may be separated theoretically at equilibrium at a certain pressure and temperature state. A small separation effect can be achieved by this, because only one equilibrium stage between liquid and vapour phase is thereby realised. Contacting again vapour and liquid flows leaving one single stage in co-current mode, no further separation effect can be achieved. Under real conditions equilibrium will not be reached, which is then expressed in calculation as tray efficiency. Increased mass and heat transport may be obtained by mixing and separation of flows from single distillation vessels working at different operating points. Such a system of several stages may also be denoted rectification, if the streams leaving the micro devices are connected in counter-current operation mode. Thereby micro devices are as individual modules representing unit operations of such a process. Modular Micro Rectification (MMR) for discontinuous phase contact consists of unit operations heating, cooling, mixing and separating. Heat exchangers, mixers and cyclones for phase separation are serially connected to counter-current rectification system with the highest mass and heat transfer efficiency.
Continuous contacting of phases for the purpose of mass and heat transfer at counter-current operation mode with the exception of membrane applications only makes sense up to now for absorption process. Advances were reported by literature for the design of continuous and also discontinuous contacting, counter-current rectification in only one single micro structured apparatus [1,2,3]. Generally continuous phase contacting counter-current micro devices can only be seen as useful without occurrence of mixing effects caused by friction forces on phase interface.
However, a plant for Modular Micro Rectification containing several unit operations offers a correspondingly large number of manipulable variables, which have to be coordinated for reasonable handling of the single devices (Fig. 2). Due to the design of micro scaled devices plants form sophisticated systems, while for a fully optimized control still no common satisfying solution exists.

When operating an electrical powered evaporator for modular rectification purposes, designed by Forschungszentrum Karlsruhe, a strong interaction of mass flow with the vapour fraction and the outlet temperature can be observed [4]. Defined operating point for mass flow, temperature and vapour fraction can only be held with difficulties using traditional methods of linear control technology. When mass flow is increased, temperature at the evaporator outlet is reduced dramatically. Rising then the power input to maintain the temperature leads due to a increase of pressure in the micro-channels, which in turn lowers the mass flow and lifts temperature excessively again.
In a narrow range around operating points for mass flow and outlet temperature a step test was performed. The resulting step responses were used to tune the PID-controllers for the coupled loops mass flow and outlet temperature (Fig. 1: coupled variables).
Time constants of the systems differ strongly from each other. For the effect of power input on the outlet temperature a dead time of ten seconds and a time constant of one hundred seconds could be revealed by the step tests.



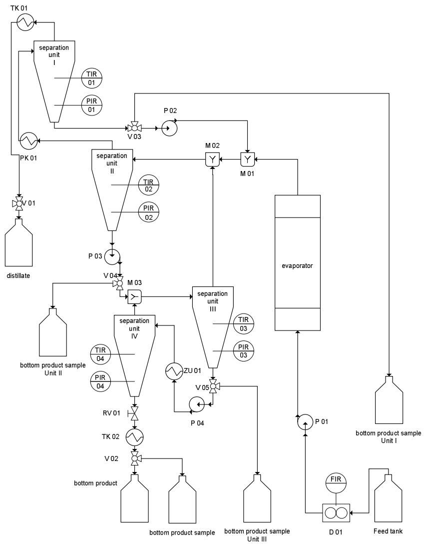




Fig. 1: Coupling of outlet temperature with mass flow displayed as linear transfer functions.
Fig. 2: Four stage Modular Micro Rectification (MMR)

The constants of the influence of pump control signal on the mass flow are determined by a dead time of only 2.6 seconds with a time constant of six seconds.

Sampling intervals of 0.1 seconds for controlled variable mass flow and one second for outlet temperature had to be chosen. Using the before determined PID-gains the system could not be operated fully stable (see Fig. 3). At mass flows or temperatures or combinations of these variables being not positioned within identified range the system performs an undamped oscillation. Due to strong action of the controllers on the system intense stress on the actuators is caused (Fig. 3).

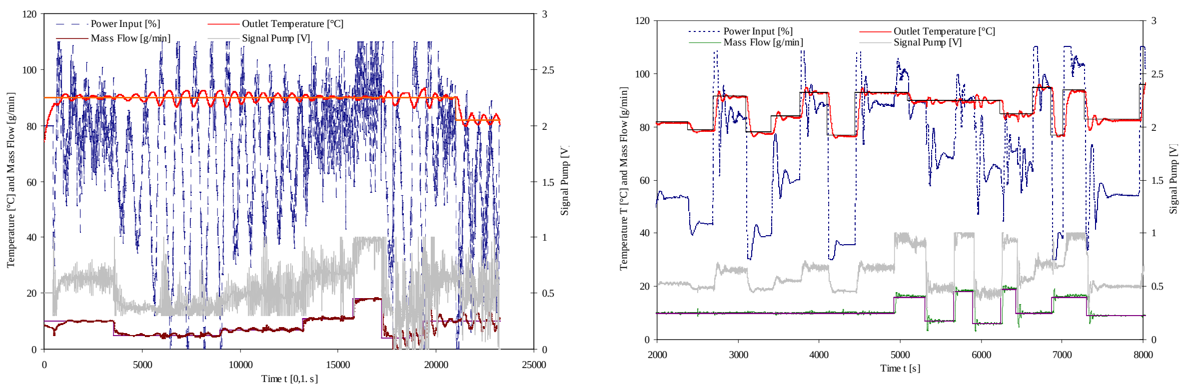



Fig. 3: Before and after Optimization of the Micro Evaporator by NMPC

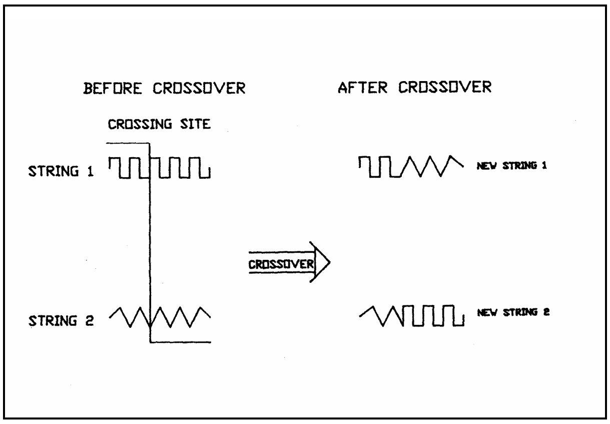
It could be demonstrated by several experiments, that precise control of the process through the use of PID-control system can be seen as a challenge. For dynamic optimization of this multi-variable evaporation process with nonlinear system dynamics the first time a Nonlinear Model Predictive Controller (NMPC) had to be applied to the field of Micro Process Engineering. MPC generally has an internal model of the complete process by which the historical trend of the process variables (feed forward, manipulated and controlled variables) is monitored and registered. Hence, it is also possible to calculate and predict future trend of controlled variables for a time horizon, when any intervention by the controller is avoided [5].

By use of optimization algorithms similar to a chess computer the best strategy for the manipulated variables is generated, thereby a control is converted to an optimization task.

To calculate an optimal control sequence for the manipulated variables, the MPC performs a minimization of energy consumption and operation costs to obtain a given objective, which is expressed by a minimal difference between set-points to actual value of the controlled variables. The square of the deviations of the controlled variables from their set-points together with action of the manipulated variables are minimized over a certain future time horizon. Such an objective function (J) for a simple **S**[ingle] **I**[nput] **S**[ingle] **O**[utput] system with by definition only one manipulated and one controlled variable may be formulated as followed [6,7,8,9]:

$$J(U,t) = P \cdot \sum_{i=N_1}^{N_2} \left[ y_R (y_R(t+i) - y(t+i) \right]^2 + \Gamma \cdot \sum_{j=1}^{Nu} \left[ u(t+i-1) - u(t+i-2) \right]^2$$

This objective function contains also a set of parameters for tuning the controller. Through coefficients Rho (P) and Gamma (Γ) the future control behaviour can be manipulated by penalizing energy consumption or otherwise reducing control efficiency. The resulting constrained cost function is non-convex making detection of relative local optimum and the prevention of suboptimal solutions a difficult task. This obstacle can only be gone around using a combination of heuristic with gradient optimization methods. Optimization of complex states like unsteady operating conditions, changing set-points or constraints, in advance is performed by genetic algorithm.



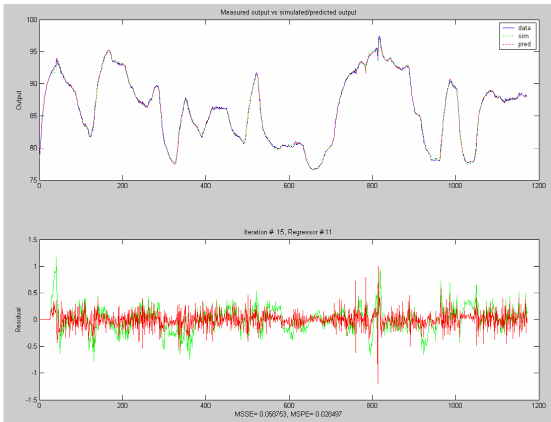




Fig. 4: Simple example for Crossover of parents producing offspring after Goldberg [10]
Fig. 5: NARX-Modelling of the outlet temperature

Genetic algorithms are as stochastic optimization methods based on the principle of natural selection and the evolutionary concept of nature. A natural parameter range of an optimization task is coded as a finite string by a limited set of characters. These search methods base upon a whole population of individuals producing an offspring by the genetic operators variation and selection, which is able to give better solution for an optimization task than their parents generation would have done. These artificial individuals are generated from the strings of a previous generation, additionally by operator mutation entirely new pieces of information are introduced (See Fig. 4). It is an efficient optimization technique that uses historical information for detection of local extrema. At unsteady operation of plant the solution vector is passed in every discrete time step by the heuristic algorithm to an implementation of gradient method of Levenberg-Marquardt, which finally performs the exact detection of the function minimum by sequential step method.

$$(J^T \cdot J + \mu \cdot \mathrm{diag}(J^T \cdot J)) \cdot h_{lm} = - J^T \cdot f \quad \text{and} \quad u_n^* = u_{n-1}^* + h_{lm} .$$

At completely stationary operating conditions the previously identified solution vector can usually be used for the initial control sequence, what directly leads to a significant reduction of CPU load.

Grouped nonlinear process models in shape of two NARX polynomials were first time implemented in a **M**[ultiple] **I**[nput] **M**[ultiple] **O**[utput] formulation of NMPC (Fig. 5: NARX: **N**[onlinear] **A**[uto]**R**[egressive] [with] [e]**X[**ogenous] [inputs]). Every training procedure a model is evolved from a set of several thousand regressors, which consist of nonlinear combinations of the lagged manipulated with the controlled and feed forward variables of the process. The total number of regressors depends on the highest power of the polynomial terms and the lag time of every variable. High polynomial order or long lag times lead directly to increased computation effort and CPU load. Various methods were proposed for the selection of polynomial structure and regressors. But until now structure selection is still not fully solved. For this work variations of the **F**[orward] **R**[egression] **O**[rthogonal] **E**[stimator] and the **S**[imulation] **E**[rror] **M**[inimization] [with] **P**[runing] methods were considered.

Using FROE algorithm the model structure is iteratively incremented until a specified prediction accuracy is obtained. Thereby parameters are estimated by means of orthogonal least squares, while the structure selection is based on the **E**[rror] **R**[eduction] **R**[atio] criterion:

$[\mathrm{ERR}]_i = \dfrac{\mathrm{MSPE}(M_i) - \mathrm{MSPE}(M_{i+1})}{\sum_{t=1}^{N} y^2(t)}$ and also $[\mathrm{ERR}]_i = \dfrac{\hat{g}_i^2 \cdot \sum_{t=1}^{N} w_i^2(t)}{\sum_{t=1}^{N} y^2(t)}$ with the corresponding model

$$y(t) = w^T(t) \cdot g + \xi(t)\,,$$

where $w_i$ is the auxiliary orthogonal regressor and $g_i$ is an estimated parameter. Because of the orthogonality of regressors $w^T(t)$, the significance of every candidate regressor can be evaluated independently.

A more effective criterion estimates the model structure on the basis of the simulation error, substituting the **M**[ean] **S**[quared] **P**[rediction] **E**[rror] with the **M**[ean] **S**[quared] **S**[imulation] **E**[rror]. The resulting criterion is then denoted **S**[imulation] [Error] **R**[eduction] **R**[atio]:

$$[\mathrm{SRR}]_i = \frac{\mathrm{MSSE}(M_i) - \mathrm{MSSE}(M_{i+1})}{\sum_{t=1}^{N} y^2(t)}\,.$$

Every iteration step the model $M_{i+1}$ is evaluated and compared to the model $M_i$ one step before. This criterion for selecting regressors is also complemented by a systematic procedure for regressor deletion, included in the training procedure to simplify the regressor selection. Not significant terms are deleted by a so called “pruning procedure“ similar to Neural Nets. A complete iteration of the SEMP algorithm either adds a new regressor to the actual model or substitutes one or more of its terms with it, with the objective to improve the performance by variation of regressors.

Every discrete time step the predictions from these polynomial models of controlled variables mass flow and outlet temperature are then evaluated numerically and integrated into objective function.

The concept was formulated generically in C++ and implemented as a **D**[ynamic] **L**[ink] **L**[ibrary] in the Process Control Software LABVIEW 7 as a MIMO formulation (Fig. 6). For editing the polynomial models also on LABVIEW **G**[raphical] **U**[ser] **I**[nterface] a parser was created.

Based on experimental results it was demonstrated, that NMPC keeps the coupled variables mass flow and temperature with minimal control activity in the entire two-phase region at their set-points. Manipulated variables are calculated in optimal ratio to each other.

As a consequence the mechanical stress on actuators and energy consumption is kept low, which reduces directly investment costs. A decrease of operating cost can easily be achieved by reduction of the amount of failure output in production process. Model mismatch caused by variation of plant behaviour or inlet composition is compensated by error minimization in closed control loop.

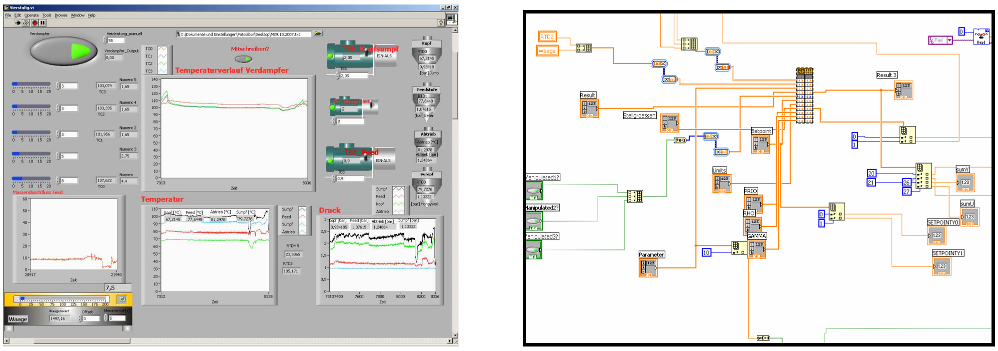


Fig. 6: Programming Interface of LABVIEW with a Library Function Node

The proposed "Nonlinear Model Predictive Control" concept has also already been successfully applied to mechanical transport systems and de-inking plants in the field of paper and pulp industry by the eposC Ltd. in Grambach near Graz (Austria). For the optimisation and production increase of twenty percent with additional reduction of chemical consumption in the paper processing of Norske Skog Bruck (Austria) the project was awarded with the INNOward 2007 of the Austrian Federal Economic Chamber in the category “Energy/Environment”.

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