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Nonlinear Model Predictive Control based on Existing Mechanistic Models of Polymerisation Reactors

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Abstract: Model Predictive Control (MPC) is established as the most powerful and most successful method for multivariable control in the process industries. Most industrial applications of MPC rely on linear dynamic process models that are identified from active experiments on the plant. If a rigorous mechanistic model of the respective process unit already exists, it would be attractive to use this model directly inside an MPC algorithm. The PSE software “gPROMS Nonlinear Model Predictive Controller” (gNLMPC) provides precisely this functionality, and this paper describes its application to a polymerization reactor. Properties, features and advantages of linear and nonlinear MPC are compared systematically.

Keywords: Model Predictive Control, Distributed Control System

1. INTRODUCTION

Across all industries, growing challenges require new solutions to optimize productivity and efficiency. Bringing automation, digitalization, and cutting-edge technologies together in a seamless way enables the comprehensive transformation of data into valuable knowledge – the next step of digital transformation. A key tool in this transformation is the innovative combination of plant data and modelling, to gain new insights and create a next generation of digital twins for plants, processes, and products.

Model Predictive Control (MPC) is established as the most powerful and most successful method for multivariable control in process industries: Qin/Badgewell (2003), Dittmar/Pfeiffer (2004) and (2006). Typical application areas are process units like distillation columns, steam crackers, fluidized bed dryers or multi-zone ovens, c.f. Pfeiffer, Grieb et al. (2014). However, most industrial applications of MPC still rely on linear dynamic process models that are identified from active experiments (like step testing) in the plant. While this approach is suitable for many continuous production processes where a linearized model describes the nonlinear plant dynamics with sufficient accuracy around a fixed operating point, it becomes tedious or unfeasible for batch processes or semi-continuous processes with multiple products and frequent grade changes, like e.g. polymerization reactors.

In contrast, if a rigorous mechanistic process model of the respective process unit already exists, having been developed for some other purpose such as an operator training system, then it would be attractive to use this nonlinear process model directly inside an MPC algorithm. Such a model not only describes process behaviour around a fixed operating point for a single product, it can also describe plant startup and shutdown, process behaviour for different products and even grade transitions from one product to another during running operation. Rigorous models are derived from balance equations for mass, energy and impulse, together with algebraic equations for phase equilibria, chemical equilibria, reaction kinetics, transport processes etc.

However, the improved predictive power delivered by a more flexible model comes with an increased computational burden; for example, some mathematical properties like the convexity of the MPC inherent optimization problem for linear process models and quadratic performance index are no longer applicable for the nonlinear case. This can make the solution of the optimization problem in real time much more challenging.

The company PSE (Process Systems Enterprise, London) is active in the area of process modelling and process simulation. Their software suite gPROMS does not only contain libraries for equation-oriented modelling of chemical processes, but also powerful mathematical algorithms to solve optimization problems. The acquisition of PSE by Siemens opens the path to integrate PSE software solutions into distributed control systems like SIMATIC PCS 7 and exploit gPROMS models during routine production operation.

Therefore, all software prerequisites are now available to venture into the emerging area of nonlinear MPC: Allgöwer, Badgwell et al. (1999), Allgöwer, Findeisen, Ebenbauer (2008). This paper describes the application of gNLMPC to an example of a continuous polymerization reactor. In the first sections of the paper, basics of MPC and gPROMS are briefly reviewed. Finally, the properties, features and advantages of linear and nonlinear MPC are compared systematically.

2. BASICS OF MPC

All MPC algorithms exploit the IMC principle (Internal Model Control, c.f. Garcia/Morari (1998)): a dynamic process model is not only used for offline controller design but constitutes an integral part of the online control algorithm, where it is used to predict future process behaviour along a specified finite prediction horizon. Typically, there are two variants of prediction used inside MPC algorithms: (1) The prediction of free response shows what the process will do if all manipulated variables (MVs) are kept constant. (2) The prediction of future with control shows what the process will do if the manipulated variables are moved in a specified way along a limited time in the future called control horizon.

The second central idea of MPC is to formulate the feedback control problem as an optimization problem: minimize the squared sum of “control deviations” and other “costs” of control like MV moves over a finite time horizon. The specific formulation of the objective function for optimization offers many degrees of freedom for controller design. Control deviations are differences between predicted process outputs and future setpoints. Different controlled variables (CVs) can be assigned weights in the performance index to reflect their relative importance to process operation. Future setpoints can be assumed to be constant, or can be designed as trajectories or tunnels, with desired time constants. Move penalties for manipulated variables in the objective function restrict controller moves to be more or less aggressive. The general trade-off between control performance and robustness of stability against model uncertainty is relevant in context of MPC as well.

The third central idea of MPC is the so called moving horizon principle and is similar to “rolling wave planning” in economics: although the optimization results contain a planning of future MV moves along the complete control horizon, only the MV values for the next sample step are actually implemented on the plant. In the next sample step, new measured values for the CVs will arrive, the predictions will be updated and new MV values will be calculated by optimization. This way, the prediction and control horizon are moved stepwise along the time domain.

The general signal flow of all MPC algorithms is sketched in Figure 1: the process model is running in parallel to the real process and is supplied with the same input signals *u(k)*, but it is part of the control algorithm. The difference between one-step ahead model prediction $\hat{y}(k|k-1)$ and measured process output *y(k)* is used as an estimate $\hat{d}(k)$ of unmeasured disturbances. Measured disturbance variables are included in the prediction model as process input variables to improve accuracy of prediction and achieve an effect similar to feedforward disturbance compensation in conventional control loops.

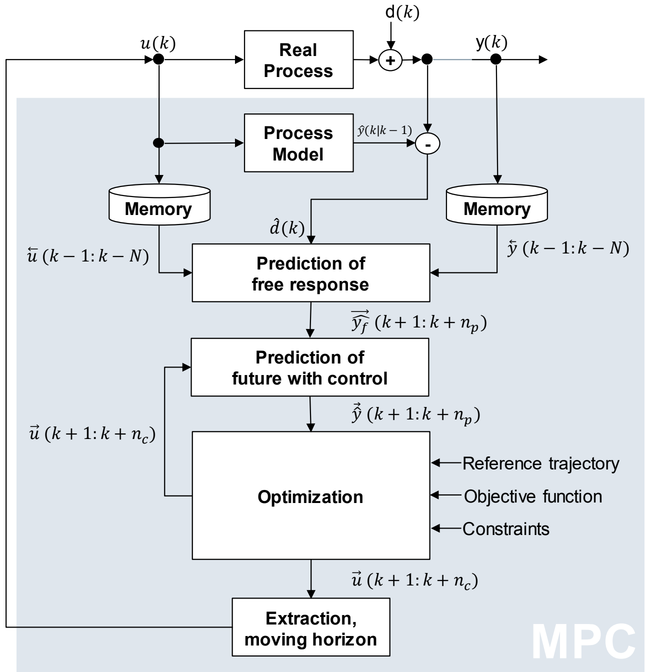

Figure 1: General signal flow for all MPC algorithms, manipulated variables *u*, controlled variables *y*. The controlled variables are predicted for the whole prediction horizon n_p , while future MV moves are only planned for discrete sample points inside control horizon n_c. Time series of future values are marked with an arrow to the right, time series of past values with an arrow to the left. Inside the brackets, the index of first and last vector element is noted.

The prediction of free response $\overrightarrow{y_f}\,(k+1\colon k+n_p)$ is calculated from the stored values of past process inputs and process outputs. The iterative optimization is visible as a closed circle in signal flow: each evaluation of the performance index for a specified set of future MV moves $\vec{u}\,(k+1\colon k+n_c)$ involves a prediction of future with control $\vec{\hat{y}}\,(k+1\colon k+n_p)$ for the whole control horizon. A lot of iteration steps of the optimization are required in each sample time of the MPC. Therefore, the computing time required for model evaluation is an important issue for MPC applications. Fortunately, most multivariable control problems of practical importance in process industries deal with slow process dynamics like quality or temperature control. Fast dynamic problems like simple flow control are typically solved by standard PID controllers inside a DCS and are included in the overall control concept as slave controllers of a master MPC. For nonlinear process models, the superposition principle is not valid. Therefore, the prediction of future with control can no longer use the prediction of free response as an intermediate result. The additive disturbance d at process output is only one example of many possible ways a disturbance can have an influence on the process.

The optimization problem is subject to constraints, namely hard constraints on absolute values and gradients of MVs. Constraints on CVs can be considered as well, but they are rather "soft constraints" like a deadband in a conventional control loop.

If the process model used in the MPC algorithm is a state space model, an observer for estimation of unmeasurable state variables is required additionally. This can only be avoided by using a pure input/output model, which is currently the state of the art in many commercial MPC software packages that rely e.g. on linear FIR (finite impulse response) or FSR (finite step response) models, e.g. Pfeiffer, Wieser et al. (2008).

3. BASICS OF gPROMS AND gDAP

The PSE gPROMS platform is a state-of-the-art software tool for modelling, flowsheeting and simulation.

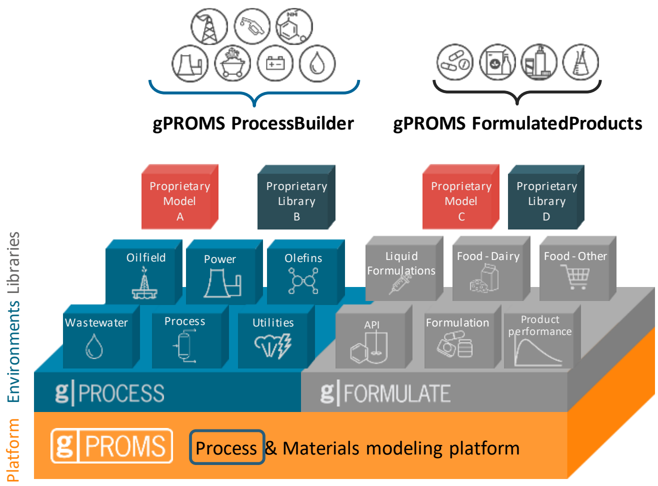

Figure 2: gPROMS process modelling platform

The gPROMS platform's powerful process modelling language allows expert modellers to create custom process models of virtually any level of complexity and validate these against experimental or plant data using built-in advanced parameter estimation techniques. Flowsheets can be built from ready-made PSE libraries, and/or user-defined custom models. These flowsheets can be deployed for either steady-state or dynamic simulations and used within PSE's optimisation capabilities. The combination of these functionalities within a single platform generates decision support based on high-accuracy predictive information in product and process innovation, design and operation.

The gPROMS Digital Application Platform gDAP is a general software platform for building, testing, deploying and troubleshooting robust, resilient and efficient digital applications that are based on gPROMS models. The platform provides general services like execution scheduling, interfaces to external data sources, data validation and storage of results. gDAP can connect as an OPC UA client to most commercial DCS platforms that provide an OPC UA server, typically as part of the central operator station server. The nonlinear MPC consists of three gDAP modules:

- Initialization: steady-state data reconciliation to cold-start the calculation
- Dynamic State Estimation
- Optimization and Prediction: solution of the optimal control problem and prediction of future trajectories

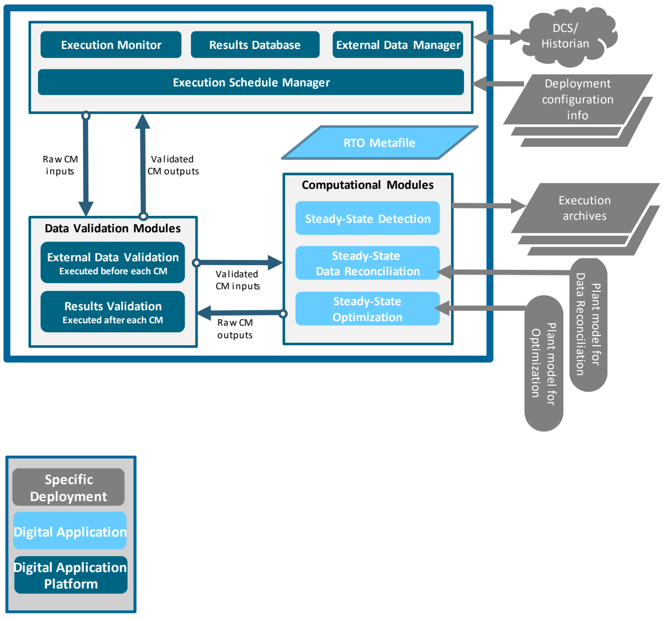

Figure 3: Components and data flow in the gPROMS Digital Application Platform

4. CONCEPT OF gNLMPC

The nonlinear MPC algorithm also follows the general MPC signal flow in Figure 1. The main difference is that the process model used for predictions is nonlinear. In the case of gNLMPC, the process is modelled in gPROMS as a DAE system of the form:

$$f(x, \dot{x}, u, d, \theta) = 0.$$

It contains a vector of state variables $\vec{x}$ and a vector of model parameters θ. The process model can (and must!) be used to estimate unmeasurable states. Additionally, if an online estimation of time-variant parameters like fouling or coking is available, the up-to-date values can be used in the model. Although the model is a continuous time DAE, the controller outputs u are considered only for discrete sample times. The formulation of the objective function to be minimized by calculation of decision variables $\vec{u}\ (k+1{:}\,k+n_c)$ is similar to the linear case. Note that in contrast to many linear MPC algorithms, gNLMPC does not work on incremental MV steps, but uses the absolute values of manipulated variables u. The objective function (Bartusiak, R.D. (2007)) used in the optimisation problem is shown below. Control deviations are formulated with respect to a CV envelope with upper and lower bounds (first line of formula), and MV move penalties are applied for controller tuning (last line of formula). In contrast to many linear MPC algorithms, absolute values of controlled variables and manipulated variables can also be included in the objective function:

$$
\min_{u_{i,k}\,|\,\lambda_i^u=1} \sum_{j\in CV} \lambda_j^z \left[\begin{array}{l} C_j^{\prime z,lo} \int_0^{T^{opt}} \max\left(0, z_j^{ref,lo}(t) - \bar{z}_j(t)\right)^2 dt \\ +C_j^{\prime z,hi} \int_0^{T^{opt}} \max\left(0, \bar{z}_j(t) - z_j^{ref,hi}(t)\right)^2 dt \end{array} \right]
$$

$$
+ \sum_{j\in CV} \lambda_j^z C_j^z \int_0^{T^{opt}} \bar{z}_j(t)dt
$$

$$
+ \sum_{i\in MV} \lambda_i^u C_i^u \sum_{k=1}^{K} \delta_k u_{i,k}
$$

$$
+ \sum_{i\in MV} \lambda_i^u C_i^{\delta u} \sum_{k=1}^{K} \left|u_{i,k} - u_{i,k-1}\right|
$$

The variables z can be measurable process outputs y or model states x. The parameters C_j^{xxx} are weights for the individual contributions to the objective function and can be specified by the user. The binary λ-parameters are used to activate or deactivate individual MV and CV channels temporarily.

Due to the nonlinearity of the process model, the objective function is no more a convex function of the decision variables. However, this dynamic, non-convex optimisation problem can be handled by the SQP optimization solvers available as standard in the gPROMS platform.

5. APPLICATION EXAMPLE POLYMERISATION REACTOR

As an application example for nonlinear MPC, a polymerisation reactor is considered. Polymerisation reactors are the home turf of nonlinear MPC because they are difficult, highly interacting multivariable control problems where the controller has to cope with a lot of different product grades, different operating points and nonlinear reaction kinetics: Bartusiak, R.D. (2007).

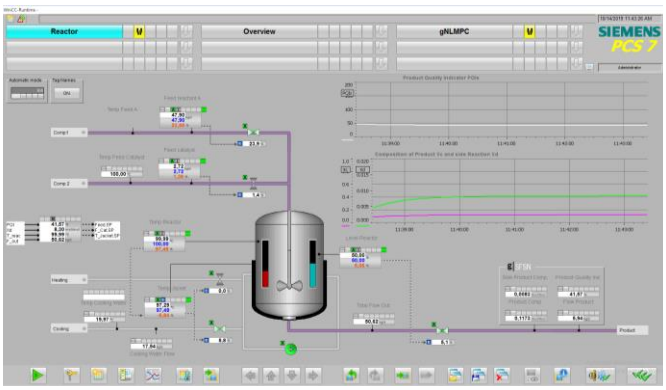

Figure 4: P&I Diagram of polymerisation reactor as shown on the operator station of a DCS (SIMATIC PCS 7)

The polymerisation reactor considered in this paper (c.f. Figure 4) is operated with continuous, PID controlled feed of gaseous monomer and feed of catalyst as a solid in suspension. Inside the reactor, long-chain polymer molecules are growing by connection of short-chain monomers, starting at catalyst particles.

Level inside the three-phase continuously stirred tank reactor is controlled via the outlet valve. Temperature inside the reactor is controlled by a cascade structure: the master controller calculates setpoints for a slave controller for jacket temperature, which manipulates heating steam and cooling water valves via a split range function. Product quality related to properties like melt flow index and density of the polymer cannot be measured directly, but is calculated by a soft-sensor which relies on a mechanistic process model as well. The concentration of an undesired side-product is also considered.

The dynamic behaviour of the polymerisation reactor is captured by a system of differential and algebraic equations:

- Mass balances for monomer, catalyst, product and side-product.
- Energy balances for reactor content and reactor jacket.
- Algebraic equations for total mass holdup, molar fractions, jacket cooling duty, reaction kinetics (of main reaction and side reaction) and product quality indicator.

The flow control loops are assumed to settle inside one cycle time of the MPC, such that their dynamics can be neglected.

The main requirements for process control are:

- achieve desired product outflow *F_Prod* (in a specified zone of flow values)
- at specified product quality *PQI*
- with minimum concentration *Xd* of side product (below specified threshold);
- keep reactor temperature *T_Reactor* in allowed range.

The following variables can be manipulated:

- Feed flow of educts (setpoint for slave controller FIC_Educt)
- Feed flow of catalyst (setpoint for FIC_Cat)
- Jacket temperature (setpoint for slave controller TIC_Jacket)

Within gNLMPC it is relatively simple to modify the control scheme, for example the combinations of manipulated or controlled variables.

It is possible to use any dynamic gPROMS model within gNLMPC, including one that has been previously developed for an operator training system. The cycle time in the case study described here is less than 1 minute. The existing base layer PID controllers, e.g. feed flow or jacket temperature controllers, that are intended to receive setpoints from the MPC, have to be included in the model. There is no need to disturb production by step tests in the real plant. Anyway, it would be impossible to perform step tests for each of the different product grades and any operating point that is relevant for such a multi-product plant.

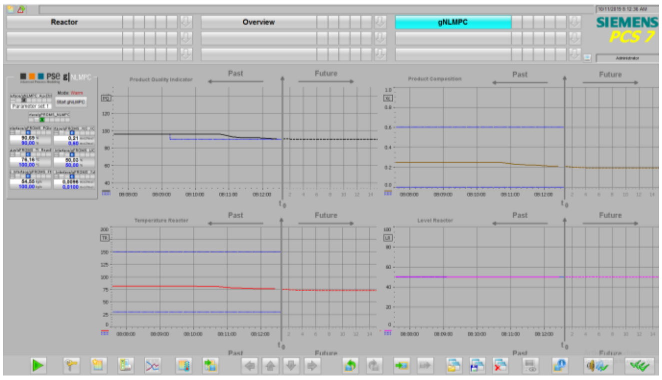

Figure 5: Automatic grade change in polymerisation reactor as a setpoint step for gNLMPC. The vertical line in each trend is the current time and future predictions are displayed to the right of this line.

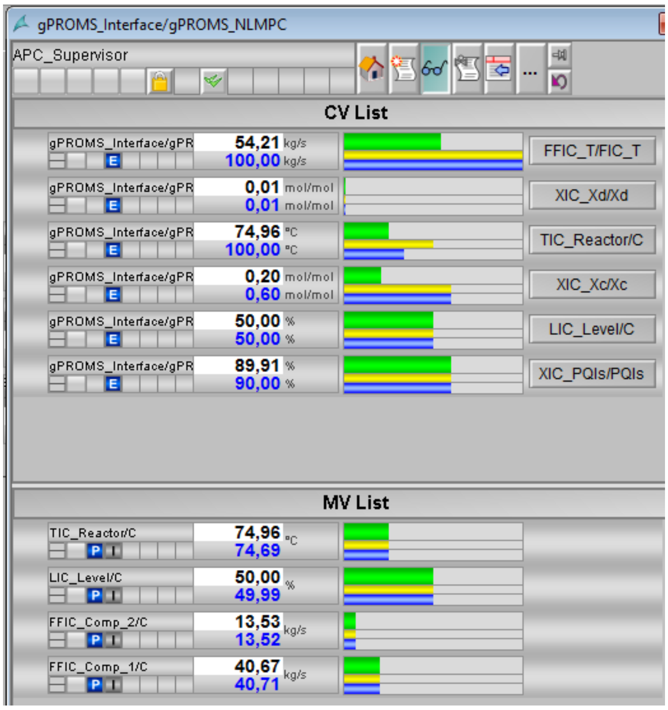

Figure 6: Overview of all MPC CVs and MVs automatically generated in operator station faceplate of APC supervisor function block of SIMATIC PCS 7

Due to the higher accuracy of predictions, NLMPC can outperform any linear MPC. The effects of external disturbances on product quality are minimized. Grade changes are treated as setpoint steps and automatically handled by the controller. Compared to the current way of plant operation, where automatic control is interrupted for grade transitions and operators have to perform this difficult task manually, the grade transitions are now run fully automatically, reproducible and time-optimal, reducing the off-spec production in between two grades.

The simulation example polymerisation reactor is available as a running software demonstrator for discussion with interested customers. In parallel, the first industrial application of gNLMPC is currently under development in collaboration with a pilot customer in the US.

6. LINEAR VERSUS NONLINEAR MPC

Important features and advantages of linear and nonlinear MPC are compared in the following tables.

Table 1: Comparison of linear and nonlinear MPC

	Linear MPC	**Nonlinear MPC**
Process model	Linear black-box I/O-model, e.g. FSR	Nonlinear mechanistic white-box model
Modelling	Identification from measurement data	Fundamental conservation laws, thermodynamics, plant data for parameter tuning
Requires…	active plant experiments, e.g. step testing	domain specific modelling know-how
Models…	work on deviations only	work on absolute values and require state observer and initialization procedures
Performance index	Quadratic cost function	Arbitrary form of cost function
Optimization problem	Convex, only one global minimum	More complex, can have local minima
Algorithm	QP-Solver	General nonlinear solver e.g. SQP
Operating range	limited by validity range of linearized model and robustness of controller	depends on predictive power of model but can be much larger than for linear models
Different products…	requires separate step tests	can be handled by model parameter variation
Grade changes…	are driven in manual mode	are considered as setpoints steps to be optimized

Table 2: Implementation aspects of linear and nonlinear MPC

	Linear MPC	**Nonlinear MPC**
Computation time	Limited, can be further reduced by simplifications	Higher, depends on model complexity, is difficult to predict a priori
Implementation	DCS-embedded ("lean MPC") or on separate PC ("full-blown MPC")	Increased computational load generally requires a dedicated PC
User-Interface	Standard faceplates (embedded) or standard APC interface blocks (full-blown)	Project-specific implementation or standard APC interface blocks
Configuration	Standard configuration software that belongs to the respective MPC package	Early stage of adoption means project-specific implementation (up to now)
Maintenance…	can be performed by automation engineers	requires modelling experts

Typical examples of linear MPC are DMC+ by AspenTech, ProfitController (alias RMPCT) by Honeywell and INCA by Ipcos, besides the DCS-embedded MPC function blocks included in DeltaV by Emerson and SIMATIC PCS 7 by Siemens. Currently there are only a few commercial software packages available for nonlinear MPC, e.g. Pavilion8 MPC by Rockwell Automation. The arguments in the tables explain why the majority of MPC applications in process industry still rely on linear models, while in special application areas running batch, semi-batch or semi-continuous processes like polymerisation or crystallisation, nonlinear MPC is on the rise.

The cost for development of first-principle models can be considerable, but over the last decades, significant progress has been made improving software tools for implementation, tuning and maintenance of such models: Pantelides (2013). Heuristics or data-driven submodels can be included if needed. The application of first principle models is especially attractive if they can be exploited for different use-cases across plant lifecycle, starting from process development via front-end and detailed engineering up to virtual commissioning and operator training. This way the investment into modelling is leveraged across plant lifecycle. The detailed model equations may be either openly accessible, or proprietary to the provider of the simulation software as part of modelling library components, or proprietary to the company who is modelling a special process they are operating themselves. The robustness of a nonlinear MPC against model mismatch depends on the aggressiveness of controller tuning, similar to any other control algorithm. For higher model uncertainty, a more conservative controller tuning is recommended. However, in cases of nonlinear processes that are not operated in a narrow domain around a fixed operating point, nonlinear MPC will profit from high-fidelity first-principle process models.

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