

# Dynamic Process Operation Under Demand Response – A Review of Methods and Tools

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Participating in electricity markets through demand response causes new requirements for optimizing process control of chemical plants. The last ten years have brought great advances in the formulation and solution of economic nonlinear model predictive control and state estimation to support operation of processes under dynamic constraints. However, gaps remain regarding the availabilities of suitable plant models capable of describing processes active in demand response as well as of robust schemes for state estimation and economic nonlinear model predictive control in commercial tools.

**Keywords:** Demand response, Dynamic process models, Economic NMPC, State estimation

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## 1 Motivation and Introduction

There is a worldwide push for increasing electricity generation from renewable energy sources to reduce greenhouse gas emissions and limit the extent of climate change. As detailed by Kätelhön et al. [1], this is a major factor for the chemical industry. As predicted, the usage of electricity by the chemical industry will increase heavily. With its increased share and growing amount of renewable electricity generation, the chemical industry will need to adjust its production processes to the electricity market. In Germany, parts of the chemical industry, which rely on electrical supply, such as cryogenic air separation or chlor-alkali electrolysis, are challenged by increasing costs for electricity and fluctuation of power generation.

### 1.1 Demand Response – Fluctuation of Steady-State Processes, Reaction to Electricity Market

In 2019, the share of renewable sources in Germany's electricity generation was at 54.3 %<sup>1)</sup> consisting of wind power (74 %), biomass (16 %), and solar (10 %). Prices varied between –25 and +75 € MWh<sup>–1</sup> in February and –50 and +125 € MWh<sup>–1</sup> in July of 2019<sup>2)</sup>. At the same time, monthly prices for intraday auctions were between 30 and 70 € MWh<sup>–1</sup> in 2019. These fluctuations endanger energy-intensive industries, however, also offer possibilities for new business models [2].

Traditionally, industrial consumers have long-term contracts to ensure low prices. Also, regulations, such as network fees (German: Netzentgelte), incentivize minimization of peak load<sup>3)</sup>. Apart from participating in the spot market, there are several further options for industry to profit from varying prices. The most talked-about is demand side management (DSM), which describes means to influence electricity consumption to complement fluctuating energy production, to stabilize electric grids, and realize cost reductions for consumers [3].

Commission Regulations (EU) 2017/2195 [4] and 2017/1485 [5] describe future schemes for control reserves and DR for the European Union. The schemes contain three types of reserves, which can be marketed: frequency containment reserves (FCR), automatic frequency restoration reserves (aFRR), and manual frequency restoration reserves (mFRR). For FCR a load change needs to be established within 30 s, for aFRR within 5 min, and for mFRR 15 min.

Given that this is a market worth billions of euros (see Fig. 1), industry and academia have started investigations into flexibilization of electricity-heavy processes. An initial emphasis is on air separation. They show a clear emphasis on scheduling [6–14], discuss operational and control

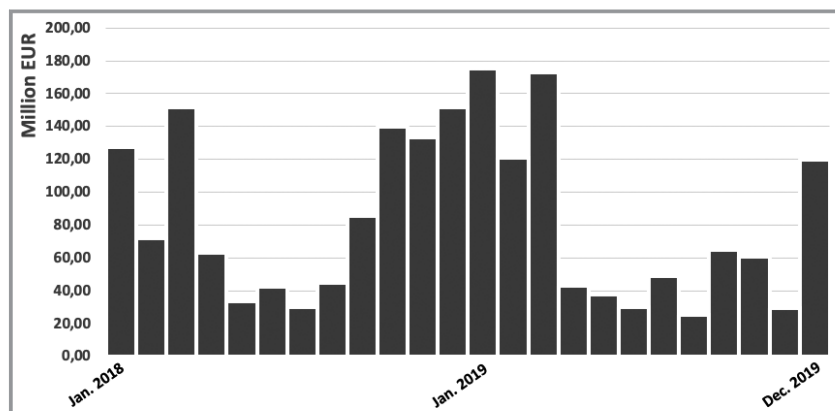
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1) [www.energy-charts.de/ren\\_share\\_de.htm?source=ren-share&period=annual&year=all](http://www.energy-charts.de/ren_share_de.htm?source=ren-share&period=annual&year=all) (accessed March 24, 2020)

2) [www.eex.com](http://www.eex.com) (accessed March 24, 2020)

3) [www.bundesnetzagentur.de/SharedDocs/FAQs/DE/Sachgebiete/Energie/Verbraucher/Energielexikon/Netzentgelt.html](http://www.bundesnetzagentur.de/SharedDocs/FAQs/DE/Sachgebiete/Energie/Verbraucher/Energielexikon/Netzentgelt.html) (accessed March 24, 2020)



**Figure 1.** Total costs of grid system stability in Germany for 2018 and 2019 in million EUR per month, data provided by Bundesnetzagentur, SMARD.de under CC BY 4.0.

aspects [15–17], investigate model reduction [18,12], and elaborate design towards flexibility [19–21]. Increasingly, electrochemical processes, e.g., chlor-alkali process [2, 22–31] and water electrolysis [32–42], come into focus.

## 1.2 Consequences for Process Operation

In research cited above, several pressing issues are detailed, which need to be investigated or for which solution approaches were proposed and need to be pursued further. These can be categorized into:

- planning and scheduling for DR,
- process operations and control,
- plant/process equipment.

Regarding planning and scheduling, new production management is required. This is a multidimensional problem: A process may have an overcapacity (see Fig. 2) available for DR. Storage is needed to fulfill demand in case of reduced production or to temporarily store overproduction. Process efficiency varies with load of processes, which also needs to be included in scheduling. Finally, the planning procedure always looks at a finite, moving horizon, on which the price of electricity and realizable profits from DR offers are uncertain.

Regarding process operation, control needs to ensure that fluctuations of process load do not degrade product quality

or violate process safety. In addition, process control can aide in speedily realizing setpoints or trajectories or ensure economic efficiency of the dynamic operation.

Scheduling and control are bounded by technical feasibility, i.e., minimum and maximum loads of plant/process equipment, the realizable speed of load changes, and the lifetime reduction of equipment subject to frequent load changes. On top of that, overcapacity and storage might need to be established, additional sensors and actuators to allow for switches between operation modes (continuous feed, no feed, plant shut-down).

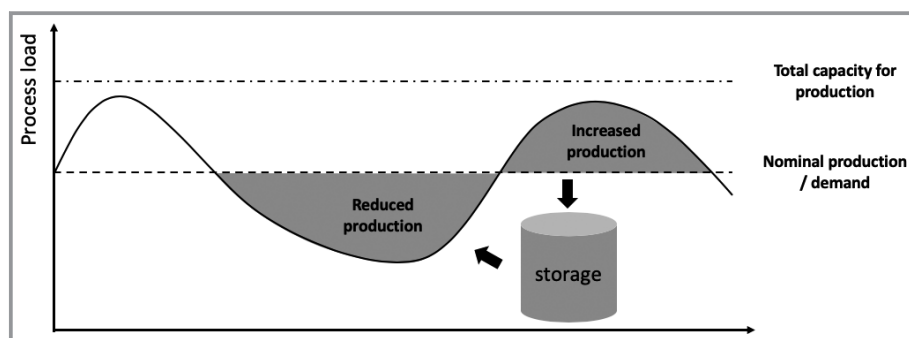
Here, focus will be on process control. We will look at methods for advanced process control, highlight recent work, and subsequently draw conclusions on requirements for further algorithmic and methodological advances.

## 2 Methods for Optimal Dynamic Process Operation

Engell and Harjunkski [43] discussed the interactions between scheduling and control and possible integrations. Here, we will focus on advanced process control separated from scheduling. The options of relevance here are summarized in Fig. 3. The focus in the following will be on the dark boxes, each of which is typically joined by a data treatment/reconciliation and state estimation block as in Fig. 4. We will briefly discuss state estimation, before going into greater depth on optimization and tracking control as well as required models to describe plant behavior accurately and with low computational cost.

### 2.1 Data Reconciliation and State Estimation

Data reconciliation and state estimation involve filtering of noise from data, detection of gross error and sensor failure, reconciliation of data to fulfill mass balances, and estima-



**Figure 2.** Basic concepts of DR.

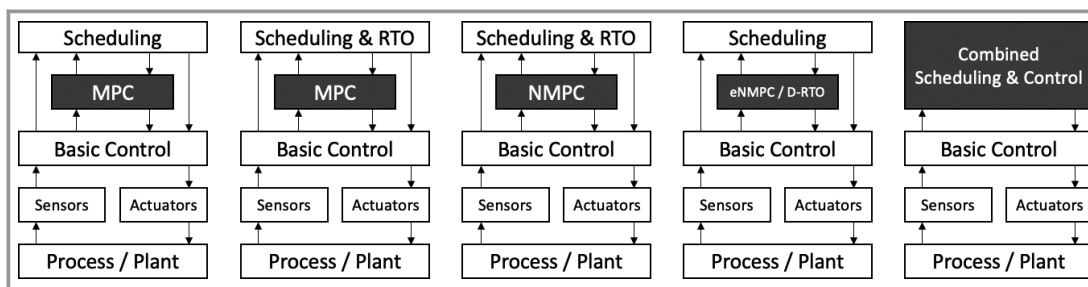


Figure 3. Various options of advanced process control in chemical processes.

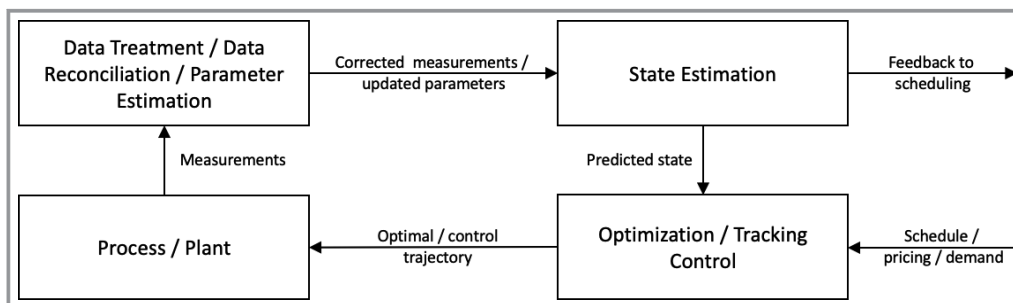


Figure 4. Interaction of plant, data treatment, state estimation, and optimization/tracking control.

tion of a future plant state based on measurement data and planned control actions. Often, data treatment and gross error detection are part of a state estimation solution. The goal is a consistent set of state variables for a future point in time, which then serves as starting point for optimization or control. Approaches for state estimation can roughly be defined into explicit and implicit methods [44].

Explicit methods usually employ predictor-corrector approaches and are dominated by Kalman filter algorithms: In a prediction a future step and its covariance are predicted based on a simulation model. In a correction step, the predicted state is updated based on current measurement data. The explicit formulation of these types of methods circumvent any necessity for an optimization step and are hence potentially more stable. Downsides of these methods are that, e.g., only one data set per estimation is used or process and measurement noise need to be known quite well to ensure reliable estimates. Variations include extended Kalman filter [44], unscented Kalman filter [45], particle filters [46], or iterative unbiased finite impulse response [47].

Implicit methods employ nonlinear programming to solve state estimation by optimization. These have a greater potential for failure or longer computation times. They allow for usage of data from multiple points in time, can connect to prior data by arrival cost and can easily be combined with filtering methods such as M estimators or fair function [48, 49]. To include measurements with highly different sampling rates, e.g., continuous measurements and rare GC samples, multi-rate implementations can be employed [50].

Existing methods for state estimation share two items, which need to be of high quality to ensure reliable estima-

tion. The first is knowledge on process and measurement noise, the second is a dynamic model of the process, which is valid for all operation conditions the plant experiences.

## 2.2 Optimal Dynamic Process Operation

This contribution focusses on layers below scheduling. This encompasses basic control, model-predictive control, and dynamic optimization with economic objectives (Fig. 3).

### 2.2.1 Integration of Scheduling and Control

As detailed in [43], there is a great need and at the same time economic potential to lift by integrating scheduling and advanced process control. However, apart from earlier work by Terrazas-Moreno et al. [51] and more recent contributions [6, 52, 53] few practical advances have been made towards this goal. Terrazas-Moreno et al. [51] investigated optimal sequencing and optimal dynamic transitions of two multigrade polymerization CSTRs. Trifkovic et al. [52] applied a two-level formulation to integrate scheduling and control. Similarly, Han et al. [53] scheduled solid oxide fuel cells and applied setpoint trajectories via linear model predictive control (MPC), while Dias et al. [6] used the formulation for air separation units. On the other hand, Caspari et al. [54] choose an economic nonlinear model predictive control (eNMPC) formulation, which includes scheduling as well as control, but avoids any integer decisions. Their application on air separation units is not yet real-time applicable, but shows a better performance compared to the two-level formulations. Alternatively, Rossi et al. [55] present an

integration strategy with an offline and an online phase. In the offline phase, a conventional campaign scheduling problem is solved, while the online phase amounts to an eNMPC formulation, which also updates the campaign schedule and avoids the solution of mixed-integer problems in real time.

There are, of course, further methodological advances on this front. Giving a detailed review of those is beyond the scope of this contribution, which focusses on the layers below scheduling in the automation hierarchy. A recent review on the integration of scheduling and control can be found in [56].

## 2.2.2 Advances in (Nonlinear) Model Predictive Control

In the integrative scheduling approaches noted above, linear MPC is the method of choice and for dynamic scheduling formulations only low order, simplified dynamic models are employed. These formulations are dynamic extensions to classical RTO-MPC, wherein real-time optimization is carried out on steady-state models and linear model predictive enacts the results.

For DR, this is insufficient as the scheduling layer needs to account for disturbances and transient behavior to ensure the computed schedule is feasible and does not lead to unreachable setpoints [57]. Also, handing control no information on the economics of the process might cause tracking of suboptimal setpoints [58]. Hence, economic nonlinear model predictive control, also known as dynamic real-time optimization (D-RTO), is a highly interesting candidate for implementing DR on chemical processes.

### *Advances in and Extensions of Linear MPC*

As noted by Darby and Nikolaou [59] linear MPC is the method of choice for constrained multivariable applications in the process industry as it is reliable, and stability is well established. Recent years have seen further extensions of linear MPC. One example is multimodel MPC, where multiple linear models of a nonlinear system are combined by a weighting method [60–62]. Secondly, Rawlings and Risbeck [63] extended MPC to discrete actuators, e.g., magnet valves. To account for changes in plant behavior, Zhao et al. [64] discuss the important topic of model updates. They introduce an error prediction technique for their model identification technique and successively update the model used for MPC. In [65] a similar technique is applied to robust MPC with parametric uncertainty. They employ online parameter estimation to improve MPC performance and reduce conservatism simultaneously.

### *Advances in (Economic) Nonlinear MPC*

NMPC both from tracking and economic optimization perspective has seen great advances. After initial implementations in the 2000s, e.g., [66, 67], focus has moved to reducing computational cost to ensure real-time capability,

investigation of uncertainty, proof of stability, and targeted formulation to ensure stability.

### *Reformulations, Transformations, Regularizations*

Full discretization of NMPC problems by orthogonal collocation, also known as the direct transcription technique, as heralded by Prof. Lorenz T. Biegler, has caused a frenzy of publications solving optimization of DAE systems by nonlinear programming (NLP). In [68] the capabilities are demonstrated on a low-density polyethylene reactor.

In [69], this approach is applied on D-RTO with a two-layer architecture. The results of D-RTO are realized by fast tracking MPC. Within the D-RTO optimization problem the MPC is represented by its Karush-Kuhn-Tucker conditions and the fully discretized D-RTO is solved as a large-scale NLP.

Within DR, larger deviations between target trajectory and current plant state can be expected. This situation is addressed in [70]. NMPC tends to behave overly aggressive under these circumstances given the often applied  $L^2$  norms. Instead, [70] suggest Huber penalties.

An essential building block of all NMPC schemes is the time horizon it is applied upon. Several groups have worked on various transformations of these horizons, adaptive methods, and discretization schemes. Examples are contributions of Würth and Marquardt [71] on transforming infinite horizon as finite, Griffith et al. [72] on adaptively updating NMPC horizon lengths online via NLP sensitivity calculations, and Yu and Biegler [73] on nonuniform discretizations.

### *Real-Time Capability of Nonlinear MPC*

One obstacle in applying NMPC online is the large computational cost, if used without further modification. Hence, dozens of contributions have readied NMPC for real-time by offline computation and online updates or by convexification.

Especially advanced step methods have gained attention. Propagated in [49], this approach has seen numerous implementations. A full NMPC problem is solved offline and sensitivities obtained from the Karush-Kuhn-Tucker conditions are used to update the optimal solution to a current plant state. Notable contributions to further this technique are [74] and [75].

In analogy, groups have followed the concept of neighboring extremal updates, leading to a two-layer formulation. Wolf et al. [76, 77] applied it to a distributed eNMPC setup. A slow eNMPC feeds its results to a fast neighboring-extremal controller, which carries out sensitivity-based updates of slow eNMPC results.

An alternative way to obtain sensitivities is suggested by Chen et al. [78], who prefer an inexact scheme in combination with a nonlinearity measure to trigger sensitivity updates.

As a different approach, Zanelli et al. [79] formulate a homotopy-based nonlinear interior point method, which

exploits successively tightened problem formulations. They show a speed-up of one order of magnitude. Apart from that, inexact schemes have been suggested in [80] allowing for offline computation of sensitivity. In addition to those, numerous alternative formulations such as move blocking [81], efficient input parametrization [82], or successive linearization [11] have been investigated.

#### *Stability of NMPC Schemes*

A persistent issue with NMPC schemes has long been stability, which is intimately linked to numerical complexity of their practical application. Most contributions have been accompanied by theoretical deliberations on stability properties, such as [83,84] for advanced step, [73] for nonuniform discretization, or [80] for their inexact scheme. Furthermore, contributions such as [85] ascertain certain stability properties by design in eNMPC formulations or establish stability for systems with cyclic steady state, like pressure swing adsorption [86].

#### *Consideration of Plant-Model Mismatch*

Most eNMPC rely on a close relationship between physical plant and model. As remarked by Bonvin and Srinivasan [87]: “In the presence of significant plant-model mismatch, the use of a fixed nominal model is typically insufficient to drive the plant to optimality.”

To overcome this, robust NMPC (see below) has been suggested or adaptive methods borrowing from machine learning (see below). Alternatively, Marchetti [88] suggested modifier adaption for real-time optimization, which has since been applied [88,90]. A key issue in these schemes is that a process can be excited to yield enough information from noisy measurements to correctly modify cost functions and constraints to drive a plant to its actual minimum.

A related technique is NCO tracking, i.e., tracking of necessary conditions of optimality, where a model of the optimal solution of an eNMPC problem is built offline and then used online with measurement data from a process to update optimum and change controls of a process [87]. Here, the availability of meaningful measurements and identification of controls essential for economic success of the process are crucial.

#### *Consideration of Uncertainty*

Connected to plant-model mismatch are concepts of robust NMPC, where model and measurement uncertainties are considered and their effects on violations of path or terminal constraints. In all robust formulations of eNMPC, a compromise is made regarding attainable objective to avoid violations of constraints. The various approaches differ in how conservative the back-off from constraints is.

The multistage scenario-based NMPC formulation has been widely investigated. Here uncertainty is handled explicitly in terms of scenarios, leading to a scenario tree, in which scenarios branch at points in time, at which uncer-

tainty of the previous period has been realized [91]. The formulation is made less conservative by allowing for recourse in the later stages of the scenario tree. Many additions to this approach have been suggested to better account for plant-model mismatch [92] or to relief exponential increase in complexity with larger numbers of uncertainties [93].

In addition, stochastic programming using chance constraints is also becoming more popular, where probability bounds are enforced to ensure constraint violations remain at a predefined level [94]. The technique has been applied to eNMPC problems, as in [95] and [96]. Quite similar to multistage, this technique suffers from exponential increase in complexity for larger numbers of uncertain parameters. To counter these effects, recent contributions have used data-driven surrogate models for fast online computations [97].

Besides, several other formulations for robust NMPC are being investigated including formulations using polynomial chaos expansion [98].

As mentioned above, the outright integration of scheduling and control is not covered by this contribution. However, there are developments in the integration under uncertainty, which are of consequence here as noted in [56]. One example is the dynamic identification of the optimal description of model uncertainty from batch to batch in [99]. They emphasize the importance of the choice of uncertain parameters to characterize uncertainty in process models and present a framework for rapid identification of the optimal set of uncertain parameters needed for formulation of stochastic online optimization problems using a combination of approximate statistical analysis and multipoint sensitivity analysis. The integration between scheduling and control is further discussed in [100], where the uncertainty involved is incorporated via multiparametric model predictive controllers, which take into account both the continuous as well as the binary scheduling decisions.

#### *Flexibility of Processes*

In the early 1980s, Manfred Morari stressed that “flexibility, operability, and control” should be included in the design of chemical processes [101]. Here, flexibility (or static resiliency) is the ability of a process to operate over a range of conditions, while satisfying the performance requirements [102]. One quantifier for flexibility has been introduced by Pistikopoulos and Mazzuchi [103] in the form of the flexibility index, which is a measure of probability that a design can be operated. Since the early works in the 1980s this has also been extended to dynamic resiliency, also including the transient states between the steady states. A recent example has been published in [104], where a dynamic flexibility analysis of a distillation column is carried out and the transient information is used to obtain a suitably flexible design.

While none of these indices measuring flexibility have yet amounted to the tools level, it is of course very important to point out how relevant flexibility is for the design of a



process using methods of advanced process control to operate under demand response scenarios.

## 2.3 Models for Optimal Dynamic Process Operation

As has been repeatedly stressed so far, a suitable model is key for success. Regarding eNMPC model adequacy has been stated by both [87] and [105] in terms of stability surrounding the process optimum.

In practice, models also need to be able to describe processes after larger disruptions, so need to cover a larger part of the possible operation region. Traditionally, models for MPC are obtained either through excitation of the plant and system identification or through first principles modeling and simplification. With respect to formulation of models for chemical processes active in DR, exceptionally little focus has been given to methodologies on formulation of adequate models usable for state estimation and eNMPC of those processes. Requirements for these models arising through DR are for instance the support of switches (transitions) between operation modes: Plants active in DR might switch from continuous operation to internal recycling or a partial shutdown. Hence, a warm start-up might also need to be carried out etc.

### 2.3.1 Recent Contributions on Dynamic Process Models for DR

Shehzad et al. [106] describe a modeling approach based on mixed integer linear constraints and nonlinear dynamic models and apply it to combined electrolysis and hydrogen storage. The mixed integer part describes discrete logical states, such as filling of storage, whereas dynamic equations describe continuous phenomena of the process, e.g., efficiency degradation.

Yu et al. [107] stress the importance of model reduction for plants directly connected to a fluctuating energy market. Describing an adsorber for carbon capture, they achieve reduction regarding time by applying nullspace projection and eigenvalue analysis. This amounts to a quasi-steady state approximation for states with fast dynamics. With respect to space, Yu et al. [107] employ proper orthogonal decomposition to obtain a reduced set of differential algebraic equations.

Orthogonal collocation is applied in [16] and [18] to reduce the number of equations in a models of distillation columns. Instead of a tray-based formulation, orthogonal collocation is used along the height. On the other hand, Hoffmann et al. [27] describe a fast, dynamic pressure-driven model for a reactive distillation column subject to load changes associated with DR. Their focus is on the smoothing of discontinuities, such as the flow over a weir or weeping and surrogate models for complex thermodynamics.

### 2.3.2 System Identification, Reduced order Models, and Surrogate Models

Apart from these tailored formulations, a lot of work has gone into model reduction and surrogate models for dynamic systems. Proper orthogonal decomposition mentioned above falls into this category. To give a detailed overview here would go too far. In any case, a lot more work has been carried out in this field regarding steady-state representations. Highly popular choices for surrogate models there are Gaussian process regression models [108] and artificial neural networks [109]. More recently, methods for adaptive sampling and training of surrogate models have been applied as in ALAMO [110] and the combination of surrogate models with detailed model parts to form gray-box or hybrid models [111].

On the dynamic side, the whole topic of surrogate modeling and reduced-order modeling can also be approached through the lens of system identification. An overview can be found in [112]. Typically, system identification is carried out on signals or measurement data obtained from an excited process to obtain a state-space representation [113] or a Wiener-Hammerstein model [114]. Increasingly, these methods are also employed to obtain surrogate models from originally complex simulation models through expensive sampling [115–117]. Rising in popularity are methods associated with machine learning (ML), e.g., artificial neural networks, which can also easily be employed to mimic dynamic systems. Recent applications include biological wastewater treatment [118] or crystallization processes [119].

## 2.4 Machine Learning Applied to Process Operation

Beyond the use of ML models, its methods are increasingly applied in chemical engineering. Particularly interesting for control is reinforcement learning, which attempts to find an optimal operating policy by repeated trials. First computational studies with promising results have been achieved for the Tennessee Eastman challenge [120]. Reinforcement learning is a model-free perspective at control and hence an early criticism was that safety requirements of chemical processes could not be enforced. Recent work by Gros and Zanon [121] has shown how eNMPC can be used as a function approximator in reinforcement learning and hence hard constraints can be enforced.

## 3 Applications of Nonlinear MPC

While there are reports of industrial applications of nonlinear MPC [122, 123], details on their extent and economic success remain scarce. Apart from academic work on air separation units, chloralkali electrolysis, and hydrogen generation, research on NMPC applications has focused on

systems with inherent dynamics. Many contributed on batch and semi-batch processes [82, 92, 95] with a strong emphasis on polymerization reactors [69, 124]. Secondly, systems with cyclic steady state [116], e.g., for CO<sub>2</sub> separation [73], were investigated.

Beyond that there are some academic applications on distillation and fermentation processes [125], crystallization [119], but nowhere near as numerous as the rest.

A little outside the typical scope of chemical engineering, more recent contributions of NMPC for the operation of systems directly connected to the electric grid can be found. These include large-scale fuel cells and batteries [53, 115, 126] and of course the huge field of load and frequency control in electric grids [127].

## 4 Review of the Status Quo and Outlook

Looking at the status quo on optimal dynamic process operation, it is apparent that lot of attention has been given to realizing NMPC for systems under dynamic constraints, but there is a gap to industrial realization of these. In the following, available methods are examined regarding their usability for DR and requirements for future developments are presented.

### 4.1 State Estimation

Regarding data treatment and state estimation, mature, performant technologies are marketed, e.g., gPROMS Digital Applications Platform by Process Systems Enterprise Ltd.<sup>4)</sup>. There are, however, limits to their application, especially regarding DR. First of all, the models available in commercial simulators are not designed for operation modes far away from the typical steady state, which DR can infer, more on this below (Sect. 4.3).

As noted above, there academic contributions dealt with multi-rate data. Most considered data at somewhat similar frequencies. Incorporation of extremely scarce quality data remains a challenge. In [50] we suggested on a two-layer implementation for moving horizon estimation. These techniques need to be made usable for actual industrial application. Especially, the interaction of these two layers needs to be investigated further to ensure stability and robustness.

Of course, this issue could be amended otherwise, in case fast quality sensors for concentrations were made available. Concentration measurements on a daily or weekly basis are not an option for a process connected to an electricity market operating in 15-min intervals and faster. In general, abundant availability of cheap sensor technology for quali-

ties, flows, levels, temperatures, and pressures would be a huge advantage. At the moment, very few sensors in industrial plants have redundant counterparts, making these processes vulnerable to sensor failure and sensor drift. Software for anomaly detection is commercially available but needs to find wider application and support by redundancy in sensors.

On top, regaining state estimation after its failure is an issue that could be caused by sensor failure or a process moving into a region not described by the model. Some of the adaptive techniques name in Sect. 2.2 include means of excitation to achieve process optimality. Similar measures need to be exploited for state.

This is closely related to aging of plants, which increases plant model mismatch or may cause structural mismatch, e.g., through blockage of pipes or deactivation of catalysts. Here, state estimation will become unreliable causing sub-optimality or even instability of the framework sketched in Fig. 4. Methods for model adaption, e.g., through re-estimation of parameters, have been investigated, but can typically not handle structural changes. There are methods for model discrimination and system identification, which could be applied here. However, these rely on large quantities of measurement data and on excitation of a process to generate information. Further research is required on how to safely introduce these measures into continuously operating production plants to achieve required model updates.

### 4.2 Frameworks for NMPC

Similar to state estimation, first industrial implementation for eNMPC or D-RTO are available<sup>5)</sup>. Performance of these is still largely unknown. Missing from these implementations are methods discussed for sensitivity-based updates or introduction of uncertainty. To this end, academic software has been published [124], [128], and more recently as part of Pyomo [75]. Especially the latter raises hope that academic ideas will soon be taken up by vendors.

Overall, fast and reliable convergence is a persistent issue, which is still tackled by tuning of algorithms and tailoring of models. More complex nonlinear models designed for DR will exacerbate this situation. In the past, methods for offline generation of optimal operation trajectories of eNMPC have been investigated. More research can be expected in this area in combination with sensitivity-based updates.

In the linear MPC domain distributed control with coordinating agents is well established. For eNMPC such schemes are not yet widely discussed. First attempts have been made, e.g. in traffic systems or energy grids [129]. An

4) [www.psenterprise.com/products/gproms/digitalapplications/platform](http://www.psenterprise.com/products/gproms/digitalapplications/platform) (accessed July 04, 2020)

5) [www.honeywellprocess.com/library/news-and-events/presentations/hug-america-2018-hcp-0301-optimization-for-real-people.pdf](http://www.honeywellprocess.com/library/news-and-events/presentations/hug-america-2018-hcp-0301-optimization-for-real-people.pdf) (accessed July 04, 2020)

application to chemical processes promises further advances in eNMPC to larger processes, where fast computation cannot be achieved in monolithic eNMPC architectures. Recently, Farina et al. presented a distributed MPC implementation, which identifies its surrogate models directly from a connection to the process simulation software DYNsIM [130].

As in state estimation, eNMPC is challenged by growing or structural plant-model mismatch. Some work is currently ongoing to exploit modifier adaption to converge to the plant's optimum. Nevertheless, this is not directly applicable to processes, which never or rarely achieve their steady state. Hence, further techniques for model adaption should be investigated (see Sect. 4.1).

### 4.3 Modeling

Besides models developed for batch units, models in process simulators are not meant for the full range of operation modes from start-up to shutdown. To move towards wide use of NMPC or large-scale application of DR in the chemical industry, this is untenable. Model libraries aiming at support of process operation need to be developed. Projects such as IDAES<sup>6)</sup> promise to take steps to relief this bottleneck, although with a clear focus on the power industry. Further work is needed and a stronger pull by industry can be observed in the numerous industrial research projects on DR.

Based on our own work on DR in air separation [12, 13] and chloralkali electrolysis [2, 27, 31, 50], we can draw requirements for such a new library of process operation models:

- Models need to describe filling and emptying of all equipments, i.e., column trays, condensers, reactors, etc.
- Given fast changes in the electricity market, these models should account for pressure equalization, i.e., be fully pressure-driven.
- Hence, actuators such as valves, pumps, compressors need to be included.
- Given various operation modes involved, phenomena need to be (de-)activated on demand, e.g., thermodynamic equilibrium relaxed in case of disappearing phases.

Regarding reduced-order and surrogate modeling to ensure computational speed, a lot has been achieved and the huge advances in the field of ML ensure that models are performant in optimization. A field for further research is dynamic surrogate models for systems with multiple operation modes. Such models exist for scheduling of steady-state systems [12] and an extension to dynamic systems could decrease the burden on smoothening models for application in NMPC.

### 4.4 Outlook

In the last ten years, DR has evolved into a large factor in electricity markets worldwide. With increased pressure to lower emissions and increase use of renewable energy, the chemical industry will increasingly feel economic pressure to lower cost by carrying out demand side management.

In this contribution, we have reviewed advances in state estimation, nonlinear model-predictive control, and modeling techniques with regard to application of demand response (DR) on usually continuously operated chemical plants. To enact these schemes on chemical processes at large, many prerequisites still need to be established, such as robust state estimation, widely available eNMPC, and most importantly ready-to-use models for flexible process operation. Beyond that, adaption techniques, e.g., for model updates in state estimation and eNMPC, need to be developed to account for changes in plants caused by aging or modifications. Available methods for fast online computation of MHE and eNMPC are not yet at the level at which they can be applied to highly complex large-scale processes and further work on offline precomputation and online updates as well as on distributed eNMPC and coordination is required.

Air separation processes and electrolysis for chlorine and hydrogen are already taking first, smaller steps towards realizing DR. For other processes with more complex dependencies to follow, the above-mentioned challenges will have to be resolved first.

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6) <https://idaes.org> (accessed July 04, 2020)





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## Abbreviations

aFRR	automatic frequency restoration reserves
D-RTO	dynamic real-time optimization
DSM	demand side management
eNMPC	economic nonlinear model-predictive control
FCR	frequency containment reserves
mFRR	manual frequency restoration reserves
MINLP	mixed-integer nonlinear programming
ML	machine learning
MPC	model-predictive control
NLP	nonlinear programming

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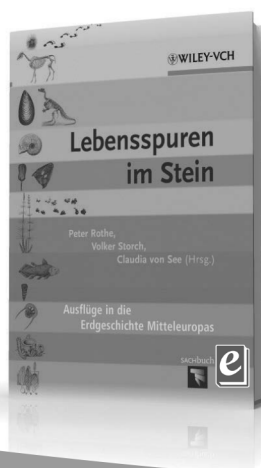
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