Novel Approaches to Online Process Optimization under Uncertainty

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The safe and optimal operation of large and complex industrial processes requires meeting goals and objectives in different time scales ranging from long-term planning and scheduling to fast corrective actions for stable operation. Realizing all the goals and constraints as a whole can be a very challenging and unrealistic task, especially if formulated as a single centralized optimization and control problem. Thus, the operation of any process is typically decomposed into various decision making layers, ranging from regulatory control, supervisory control, real time optimization, and planning and scheduling [29, Ch.10], [5].

The main focus of this thesis is the real-time optimization (RTO) layer. The economic optimization of any process performance in the context of real-time optimization is becoming more crucial in the face of growing competition, increasing demands, and the necessity to focus on sustainability and energy efficiency. Process optimization directly enables safe operation, cost reduction, improving product quality and meeting environmental regulations and this is the main focus of the RTO layer.

In many process control applications, real-time optimization uses *nonlinear steady-state* process models to compute the optimal setpoint at steady-state operation [27]. The justification for using steady-state models is twofold; 1) the economic operation of the plant often occurs at steady-state operation, 2) steady-state models are more easily available and can be much simpler [27]. RTO is also provided with constraints such as process and equipment constraints, storage and capacity constraints, product quality constraints etc. In addition, RTO uses an economic model that constitutes the cost of raw material, value of the products, operational costs, environmental regulations etc. to evaluate the economics of operation.

Traditionally, RTO implementation is based on steady-state nonlinear models that are parameterized by a set of unknown or uncertain parameters, which are updated using measurement data. The updated model is then used to compute the optimal set of decision variables by solving a numerical optimization problem. The repeated identification and optimization scheme using steady-state models is used in many commercial RTO software packages [2].

Despite the economic benefits and promises, traditional real-time optimization is not used commonly in practice. Consequently, the full potential of RTO is not exploited in process industries. The main research question that this thesis deals with is,

"Why is traditional real-time optimization not commonly used in industry, and how can these challenges be addressed?"

Challenges with traditional RTO

The main challenges which limits the industrial use of RTO include:

- **Challenge 1** - Cost of developing the model (offline).
- **Challenge 2** - Model uncertainty, including wrong values of disturbances and parameters (online update of the model).
- **Challenge 3** - Numerical robustness, including computational issues of solving optimization problems.
- **Challenge 4** - Frequent grade changes, which makes steady-state optimization less relevant.
- **Challenge 5** - Dynamic limitations, including infeasibility due to (dynamic) constraint violation.
- **Challenge 6** - Problem formulation - choosing the right formulation for the right problem.

In this thesis, we take a detailed look at these challenges and aim to address each of the challenge. The different challenges, along with the solutions proposed in this thesis for each challenge is described below.

Challenge 1: Cost of developing model

The cost of developing a model is the biggest bottleneck in the traditional RTO paradigm. Developing good first principle-based models is often challenging and expensive, especially for new application areas with limited domain knowledge. In addition, lack of knowledge or model simplification lead to mismatch between the physical models used in the optimizer and the real system. With increasing complexity of many industrial processes, simplified first-principle models are insufficient to accurately capture the system behavior.

Proposed solution: Model-free optimization approaches such as extremum seeking control as proposed in Chapter 5 may be used to circumvent the need for developing complex models. In addition, Chapter 4 proposes a systematic approach to using classical feedback controllers and simple logic structures to switch between active constraint regions. Machine learning approaches may also be used to address this challenge as briefly discussed in Appendix M.

Challenge 2: Online update of the model

Since traditional RTO uses steady-state models, the model adaptation step must be carried out using measurements that corresponds to steady-state operation. A steady-state detection algorithm is used to detect if the process is operating at steady-state conditions. This is known as steady-state wait time. In a recent review paper on current practices of RTO, [4] concludes that a fundamental limiting factor of RTO implementation is the steady-state wait-time associated with the online update of the model. If the process is frequently subject to disturbances, or if the settling times are rather long, this can lead to the plant being operated in transients for significant periods of time. With the inadequacy of steady-state conditions, the model is not updated frequently, leading to wrong values of disturbances and parameters in the model. Consequently the plant is operated suboptimally for long periods of time.

Proposed solution: To address the problem of steady-state wait time, several different approaches are proposed in this thesis. In Chapter 2, we propose a "hybrid" combination of steady-state and dynamic RTO approach, where transient measurements are used in the traditional two-step steady-state RTO paradigm. In addition, this thesis also proposes different alternative approaches to RTO that use transient measurements. For example, a novel model-based gradient estimation scheme using transient measurements is proposed in Chapter 3, that does not require the steady-state wait time. Chapter 5 proposes a novel dynamic extremum seeking scheme using transient measurements that results in a significantly faster convergence to the optimum, since it does not require the *static map* assumption (unlike most extremum seeking schemes). Additionally, the different methods proposed in Chapters 4 and 6 also use transient measurements, hence eliminating the need for steady-state wait time.

Challenge 3: Computational issues and numerical robustness

Solving numerical optimization problem to compute the optimal setpoints, leads to high computational effort. Although the computational cost is considerably less for solving steady-state optimization problems than dynamic optimization problems, the optimization problem may still fail to converge for large-scale processes (numerical robustness). Therefore, there is a clear need to develop alternative approaches to RTO that does not require solving numerical optimization problems online.

Proposed solution: To avoid solving numerical optimization problems online, we propose to convert the steady-state optimization problem in to a feedback control problem, where the inputs are directly manipulated based on the feedback measurements. The Hybrid RTO approach in Chapter 2 is converted to a feedback problem in Chapter 3. A systematic approach for using classical feedback controllers along with advanced control elements such as selectors is proposed in Chapter 4, which avoids the need for a separate optimization layer. Extremum seeking control proposed in Chapter 5 and the combination of extremum seeking control and self-optimizing control in Chapter 6 are also based on feedback control.

Challenge 4: Frequent grade changes, which make steady-state optimization less relevant

Processes with frequent changes in feed, product specifications, market disturbances, frequent grade transitions, cyclic operations and batch processes etc. make traditional steady-state RTO less relevant. Such cases require dynamic optimization methods (e.g. Dynamic RTO or economic NMPC). However, solving dynamic optimization problems are computationally intensive, even with today's computing power (cf. Challenge 3). This challenge grows even more in the presence of uncertainty. In this case, one cannot avoid solving numerical optimization problems. Hence, there is a need to address the computational cost of solving dynamic optimization problems [3, 6].

Proposed solution: In the presence of uncertainty, this thesis first considers what is a good problem formation for dynamic RTO under uncertainty in Chapter 7, where multistage scenario-based formulation is identified as an effective way of handling uncertainty in the dynamic RTO problem. One of the main challenges with the multistage problem formulation is that it leads to a large problem size. Algorithms proposed in Chapters 9 and 10 deals with addressing the computation time of multistage economic NMPC by using decomposition methods and parametric optimization concepts.

Challenge 5: Dynamic limitations, including infeasibility due to (dynamic) constraint violation

The optimal solutions computed by the optimization layer is often provided as setpoints to the controllers in the automation layer. It may happen that the setpoints are not feasible for the lower level controllers, and may violate the constraints dynamically. This may be due to the unmodeled effects in the optimization layer or due to the multivariable coupling between the different control loops that are not taken into account in the optimization layer.

Proposed solution : This challenge can be addressed by using a setpoint tracking NMPC in the supervisory control layer for multivariable constrained control as shown in Chapter 2.

Challenge 6: Problem formulation - choosing the right formulation for the right problem

Problem formulation is probably one of the most important, and conceptual challenges with online process optimization. With developments in different alternative approaches to process optimization, ranging from traditional model-based formulation, to economic MPC, extremum seeking control, classical feedback control, modifier adaptation etc., a proper understanding of the advantages and disadvantages of the different approaches is lacking. Often, the different approaches are seen as competing to one another. There is no single available formulation that addresses all the challenges above.

Industrial processes differ in their infrastructure (available sensors and manipulators, computational platforms etc.), value chain (which affects the objective function) and safety criticality (robustness vs. performance) to name a few. For example, in many applications, the economic gain by using dynamic optimization may be negligible, while in others it may not be. In general, there is a lack of consensus in the literature on the use of steady-state versus dynamic problem formulation. Some applications may call for fast disturbance rejection, while some other applications can tolerate disturbances for a longer period of time. In the presence of uncertainty, some applications may require hard robust constraint satisfaction at the cost of conservativeness (safety criticality), while it may not be the case in some other applications. Understanding the needs of the application at hand, and choosing the right formulation is therefore a key factor in successful industrial application of real-time optimization.

Proposed solution: The different approaches to RTO are not contradictory, but indeed complementary. This is demonstrated in Chapter 6 using self-optimizing control and extremum seeking control. Furthermore, in the conclusion section, we attempt to provide an overview of the different approaches, comparing the advantages and disadvantages of the different approaches, in the hope that this might serve as a guideline/cheat-sheet in choosing the right problem formulation. Chapter 7 particularly considers the problem formulation of economic NMPC under uncertainty and proposes the multistage scenario-based formulation as one of the promising alternatives, that provide a certain degree of flexibility in the problem formulation.

Challenges related to human aspects

When considering the research question "*Why is traditional real-time optimization not commonly used in industry?*", one cannot ignore the human aspects. Besides the different technological challenges discussed above, one of the main bottlenecks to widespread application of real-time optimization, arises from human aspects that include the end-user's ability to learn, understand, and use the technology over a prolonged period of time. A recent industrial survey published in the International Federation of Automatic Control (IFAC) newsletter [26] aptly identifies *people* and *human aspects* as one of the major components when addressing challenges related to adopting new technology. This is also pointed out by several researchers in the field of process control and optimization, see for e.g. [6, 23, 22] to name a few. Indeed, most practitioners will also point to challenges related to human aspects as the most important among all the challenges listed here. The human aspects can be broadly divided into corporate culture and technical competence.

Corporate culture : Corporate culture forms the foundation of how an organization works, and plays a vital role in adopting a new technology. The corporate culture in some organizations may be such that, major changes such as deployment of new technology are resisted. Instead, one prefers "trusted" technology in order to minimize liability [23]. "Operator confidence" is another important aspect, as they are the end users. Failure to gain operator confidence will lead to an unsuccessful implementation of the technology.

Technical competence : Lack of competence and training is another major issue when adopting advanced optimization tools. Models and optimization tools require regular maintenance and retuning, in order to sustain the performance improvements. For example, changes in feed conditions, instrument and equipment degradation and changes in process equipment leads to performance degradation over time. The expected benefits from using online optimization tools are at a risk, without regular monitoring and maintenance [6]. This was also pointed out on a special report on process control in the Oil and Gas Journal [28].

Since the optimization layer is generally a multivariable and large-scale problem, the complexity and the understanding of the optimization concepts presents key challenges for the end users, as also previously pointed out by [24] and [21]. Often, expert knowledge is required to perform the maintenance, which may be limited in the organization[1]. With increasing number of applications, there is a paucity of skilled engineers to provide maintenance and support, to sustain the benefits. As noted by [6], skilled engineers involved in the initial implementation are often not available for maintenance, resulting in performance degradation, and the application being turned off by the operators.

Therefore, when addressing the different challenges listed above, it is imperative to take into account the human aspects. The different methods proposed in thesis are also influenced by the challenges related to human aspects. The use of simple PID control tools for optimal operation proposed in Chapter 4 is the perfect example of this, since it is based on classical control tools and simple logic blocks that have been in use for several decades in the process industry. In Chapter 7, we again consider the human aspects when justifying the multistage formulation as a promising approach to dynamic optimization under uncertainty.

Main contributions of the thesis

The thesis comprises of 10 main chapters divided into two parts.

Part I (Chapters 2 - 6) - The first part of the thesis deals with optimal steady-state operation and looks into how transient measurements can be used in order to address the steady-state wait time problem. In addition, it also presents some algorithms to achieve optimal operation without the need to explicitly solve numerical optimization problems online. To address the challenge of developing models, some model-free optimization tools are also presented in Part I. In general, Part I of this thesis deals with the use of "simple" tools for RTO, that are motivated by industrial needs.

Part II (Chapters 7 - 10) - The second part of the thesis deals with dynamic optimization problem, and in particular addresses the problem of computation cost of solving the economic NMPC problem. To handle uncertainty in the economic NMPC problem, we consider the multistage scenario-based problem formulation, which we propose to solve using primal decomposition, in order to ensure close-loop implementation.

The main contributions of this thesis are the novel methods and algorithms that are proposed in the different chapters to address the challenges listed above.
The key contributions (theory in bold and application in italics) are now listed chapter-wise:

Chapter 2 (Based on the article published in [11])

- **Hybrid RTO approach with dynamic model update and steady-state optimization to avoid steady-state wait time.**
- *Application - Demonstrated using an oil and gas production optimization problem with 2 wells in the chapter and 6 wells in [19].*

[1] This is also my first-hand experience from Statoil.

Chapter 3 (Based on the article published in [15])

- **A novel gradient estimation algorithm using nonlinear models and transient measurements.**
- *Application - Demonstrated using a CSTR process with 2 components in the chapter. This method was also successfully tested on a 3-bed ammonia reactor example [1], oil and gas production optimization with 2 wells [13] and 6 wells [7], evaporator process [14], isothermal CSTR with 4 components [17], which are all appended to this thesis.*

Chapter 4 (Based on the articles published in [17, 7])

- **Linear gradient combination as optimal controlled variables.**
- **Systematic approach to designing selectors for CV-CV switching .**
- *Application - Demonstrated using a CSTR process with 2 components and an oil and gas production optimization problem with 6 wells, and an isothermal CSTR process with 4 components in the chapter. The appendix includes an experimental evaluation of this approach for optimal operation of an electrical submersible pump lifted well.*

Chapter 5 (Based on the article in-preparation [16])

- **Novel dynamic extremum seeking scheme with fixed linear dynamics for Hammerstein systems.**
- **Bounds on neglected linear dynamics for robust stability.**
- *Application - Demonstrated using a pressure oscillation damper in lean burn combustors.*

Chapter 6 (Based on the article published in [30])

- **Hierarchical combination of extremum seeking control and self-optimizing control for improved performance.**
- *Application - Demonstrated using a 3-bed ammonia reactor example.*

Chapter 8 (Based on the articles published in [8, 9])

- *Application - Application of multistage scenario-based MPC to an oil and gas production optimization problem.*

Chapter 9 (Based on the articles published in [12, 10])

- **A Distributed multistage scenario MPC framework using primal decomposition to ensure feasibility of the non-anticipativity constraints.**
- **A backtracking algorithm to choose the step-length in the master problem.**
- *Application - Demonstrated using a CSTR process with 2 components in the chapter, in addition to an oil and gas production optimization problem [10], which is appended to the thesis.*

Chapter 10 (Based on the article published in [18])

- **A sensitivity-based distributed multistage scenario MPC to reduce the number of NLPs that needs to be solved.**
- *Application - Demonstrated using a CSTR process with 2 components.*

In addition to the different methods and algorithms proposed, perhaps one of the important contributions of this thesis is that it aims to provide an overview and a clear understanding of the different approaches to online process optimization, which is summarized in Table 2.

Although chapter 7 does not present any novel material, it presents useful and interesting discussions on optimization problem formulation under uncertainty. In particular, it provides discussions on *"What is a good problem formulation to handle uncertainty in dynamic RTO and economic NMPC?"* and provides a clear distinction between open-loop and closed-loop optimization.

Some other minor contributions include:

- A systematic approach to select the discrete scenarios for multistage NMPC from historical process data using principal component analysis (see Appendix K).
- Algorithm to shrink the uncertainty set online using recursive Bayesian weighting for time-invariant parametric uncertainty in the context of multistage scenario MPC (See Appendix L)

Industrial relevance and impact

Table 1: Control technologies used in this thesis, along with its impact based on the industrial survey from the 2019 IFAC newsletter[26]

Control Technology	Current Impact	Future Impact	Used in Chapter
PID control	91%	78%	3,4,6
System Identification	65%	72%	5
Estimation and filtering	64%	63%	2,3,8
Model Predictive Control	62%	85%	2,7–10
Process Data Analytics	51%	70%	App M,L
Fault detection	48%	8%	–
Decentralized/coordinated control	29%	54%	9,10
Robust Control	26%	42%	–
Intelligent Control	24%	59%	–
Nonlinear Control	21%	42%	–
Discrete-event systems	24%	39%	–
Adaptive Control	18%	44%	–
Repetitive Control	12%	17%	–
Other advanced control	11%	25%	–
hybrid dynamical systems	11%	33%	–
Game theory	5%	17%	–

As mentioned earlier, the main research focus of this thesis is motivated by the realization that real-time optimization is not used as much in practice as one would expect. We consider the different challenges in detail and provide various solutions to address the different challenges listed above. Furthermore, the use of simple PID controllers for optimal operation proposed in Chapter 4 may be immediately applicable in practice, since this is based on classical feedback controllers and simple logic blocks that are used widely in process industries.

The different approaches and algorithms proposed in this thesis are based on control technologies that have a high impact on industry. In April 2019, the industrial committee of the International Federation of Automatic Control (IFAC) published a list of control technologies along with its current and future impact [26] (A survey article with very similar conclusion was also published in the IEEE Control Systems Magazine [25]). Comparing the survey results in [26, 25], it can be seen that the different methods and algorithms proposed in this thesis are in fact based on the top five control technologies listed in this survey. This is shown in Table. 1, which is indicative of the industrial relevance and impact of this thesis, now and in the future.

List of publications

Over the past three years, this PhD work has resulted in 11 journal papers (8 published, 1 under revision, and 2 in-preparation) and 19 peer-reviewed conference papers (17 published and 2 under review) and more than 17 abstract-only/invited presentations at workshops and meetings. The full list of publications and presentations can be found in the authors CV.

The work has been published in high quality journals such as Industrial & Engineering Chemistry research [15, 17], Journal of Process Control [12, 30], Computers and Chemical Engineering [11], Control Engineering Practice [7], IEEE Control System Letters [18] and Processes [8], in addition to papers in well established conference series such as ESCAPE, IFAC DYCOPS, IFAC ADCHEM, and ECC, to name a few.

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Table 2: Overview and evaluation of the different approaches to online process optimization

	self-optimizing control^a (Ch. 6)	classical adv. control (Ch. 4)	extremum seeking (Ch. 5,6)^b	Feedback RTO (Ch. 3)	steady-state RTO (Traditional)	Hybrid RTO (Ch. 2)	economic NMPC/ DRTO (Ch. 7-10)^c	Modifier adaptation [20]
Cost Measured	No	No	Yes	No	No	No	No	Yes
Model	static model used offline	Only for unconstrained DOF^k	Model-free	dynamic model used online	static model used online	static and dynamic model used online	dynamic model used online	static model used online
perturbation	No	No	Yes	No	No	No	No	Yes
Transient measurements	Yes	Yes	No/(Yes^h)	Yes	No	Yes	Yes	No
Long-term performance	near-optimal	Optimal	Optimal^{e,i}	Optimal^d	Optimal^{d,f}	Optimal^d	Optimal^d	Optimal^{e,i}
Convergence time	very fast	very fast	very slow^{e,h}	fast	slow^f	fast	fast^g	very slow^{e,h}
Handle change in active constraints	No	Yes^j	No	No	Yes	Yes	Yes	Yes
Numerical solver	No	No	No	No	static	static	dynamic	static
Computational cost	very low	very low	very low	low	intermediate	intermediate	high	intermediate
Process size	small-scale	small-scale	small-scale	medium-scale	large-scale	large-scale	large-scale	medium-scale^l

^{a} SOC is complementary to the other methods that should ideally be used in combination.
^{b} NCO tracking also has similar properties but can also track changes in active constraints in addition.
^{c} Economic NMPC typically has non-economic control objectives in addition to the economic objectives in the cost function, whereas DRTO has only economic objectives. Studied in more detail in Part 2 of this thesis.
^{d} Converges to model optimum. Converges to the true plant optimum only if model is structurally correct.
^{e} requires time scale separation between system dynamics, dither and convergence. Sub-optimal operation for long periods following disturbances.
^{f} Slow due to steady-state wait time. Sub-optimal operation for long periods following disturbances.
^{g} limited by computation time.
^{h} Transient measurements can be used for gradient estimation if local linear dynamics are included as proposed in Chapter 5, resulting in reduced convergence time by one order of magnitude.
^{i} Converges to the true plant optimum and not the model optimum.
^{j} Need additional logic blocks as presented in Chapter 4. Ok for smaller problems.
^{k} Often not used in practice, instead engineering intuition is used to select suitable controlled variables for unconstrained DOF.
^{l} limited by plant gradient estimation.