Towards A Unifying Framework Blending RTO and Economic MPC

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Abstract

Nowadays, Real-Time Optimization (RTO) and nonlinear as well as linear Model Predictive Control (MPC) are standard methods in operation and control of process systems. Hence there exists a good understanding of how to combine RTO and set-point tracking MPC schemes. However, recently there has been substantial progress in analyzing the properties of so-called *economic* MPC schemes.

This paper proposes a conceptual framework to blend ideas from (output) modifier adaptation and offset-free economic MPC with recent results on economic MPC without terminal constraints. Specifically, we leverage recent insights into economic MPC based on turnpike and dissipativity properties of the underlying optimal control problem. Interestingly, the proposed scheme alleviates the need for a dedicated computation of steady-state targets by exploiting the turnpike property in the open-loop predictions. Two detailed simulation examples show that the proposed schemes delivers excellent performance, while being conceptually much simpler.

Introduction

The operation of process systems is facing steadily growing efficiency requirements driven by economical considerations. In other words, *the goal of optimal process operations is to maximize profit*,[1] which, for example, in view of the discussion on CO_2 certificates and regulations also implicitly includes ecological aspects. Hence for several decades there have been tremendous research efforts and progress on *attempting to synthesize a feedback optimizing control structure, [...] to translate the economic objective into process control objectives*.[2] Hence nowadays in industry a hierarchical approach composed of scheduling, Real-Time Optimization (RTO) and advanced control prevails.[3,4]

In case of RTO so-called Modifier Adaptation (MA) approaches[5–7]—whose origins can be traced back to[8,9]—have received considerable attention. The conceptual idea of MA is using first-order correction terms that enforce matching the plant KKT conditions (i.e. plant optimality) upon convergence. It can be shown that the MA approach exhibits significant advantages over the conventional two-step procedure of sequential parameter estimation and model-based optimization; i.e. MA allows handling structural plant-model mismatch. Recent progress includes convergence analysis based on higher-order corrections,[6,10,11] dimensionality reduction by means of directional subspace projections,[12,13] exploitation of interconnected system structures[14] and so-called nested approaches.[15] We refer to[6] for a recent MA overview. However, one limitation of MA is that—except for periodic and batch operations—obtaining gradient information of transient processes can be quite difficult.

Given the industrial success of Model Predictive Control (MPC),[16] which was mostly incubated and driven by the process industries since the late 1970s, it cannot be surprising that there exists a mature body of literature on how to combine/coordinate RTO and MPC layers.[17–21] Typically, the (static) RTO layer and the MPC layer are combined such that the former provides (static) setpoint targets to be tracked by the latter.[3,22–24] However, all these works consider so-called *tracking* MPC formulations (TMPC), i.e. MPC tailored to track a given target by minimizing the distance in receding-horizon fashion.

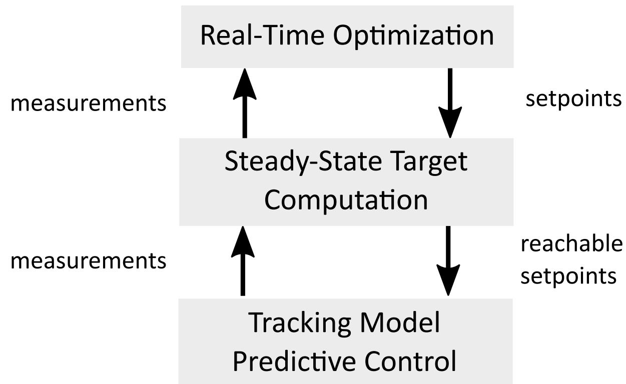

Figure 1: Typcial combination of RTO and MPC layers.

Thus, in conventional combinations of RTO and MPC one has to ensure that the setpoint targets are reachable by the MPC and, hence, a steady-state target computation is typically added as a coupling layer between RTO and MPC, cf. Figure 1. This layer can add substantial complexity to the RTO-MPC interaction, see e.g.[24] Moreover, in many industrial applications, while RTO uses a static detailed nonlinear model of the process, MPC often uses a linear(ized) dynamic model and which is, in general, not necessarily consistent with the RTO static model. Therefore, in order to track the setpoints without offset despite plant/model mismatch, MPC algorithms require augmenting the model with integrating states which are estimated along the nominal model states using plant output measurements. This leads to so-called offset-free TMPC structures.[25,26]

Recently, there have been ongoing efforts in the MPC community to analyze the behavior of so-called *Economic* MPC (EMPC) schemes, i.e. MPC formulations where the performance criterion to be minimized is not directly related to the distance to a given setpoint.[27–34] Indeed economic MPC can be seen as one approach towards Dynamic RTO (DRTO).[35] Despite the recent breakthroughs in analyzing economic MPC schemes, the handling of uncertainties and the integration of EMPC into the established hierarchical control structure still pose open problems, see[36,37] for the former and[38–40] for the latter.

Interestingly, there is close connection between offset-free TMPC[26] and constraint adaptation RTO,[41] given that both approaches add bias terms to state/output predictions in the former and to constraint functions in the latter. Moreover, in both approaches these biases are computed as the (filtered) difference between plant and model outputs. Nonetheless, the literature has not yet established and analyzed such a connection in detail.

The present paper proposes a framework to blend concepts from RTO based on MA with recent developments in the area of EMPC. Specifically, we consider the offset-free formulation for modifier-based EMPC.[39,40] We combine this approach with recent results on EMPC without terminal state constraints,[34,42] which in turn rely on the occurence of a turnpike property in the underlying open-loop optimal control problem.[43] In other words, we construct an offset-free modifier-based economic MPC, which upon convergence will guarantee plant optimality. In contrast to[39,40] we avoid the terminal state constraint in the MPC layer. Moreover, removing this constraint from the OCP alleviates the need for solving any optimization problem at the RTO level. Instead the main task of the RTO layer will be the estimation of plant gradients. Hence the main advantage and contribution of this paper is showing that there is no fundamental need for an optimizing RTO layer. Indeed under suitable assumptions—mainly availability of plant gradient information, presence of a turnpike property in the underlying OCP—the proposed offset-free modifier-based EMPC without terminal constraints can be expected to deliver equivalent performance while being conceptually much simpler.

In the present paper, we focus mostly on the underlying conceptual ideas and not on rigorous mathematical proofs. Instead we will provide condensed summaries of the already existing results, while limiting the mathematical technicalities to bare necessities. The notational convention used in the present paper is summarized in Table 1.

Table 1: Notation overview of subscripts and superscripts.

Element	Meaning	Element	Meaning
$(\cdot)_p$	plant quantities		
$(\cdot)_k$	time index of plant	$(\hat{\cdot})$	estimated quantities
$(\cdot)_i$	time index of MPC predictions	$(\cdot)^\star$	optimal values of quantities
$(\cdot)_j$	index of RTO iterations	$(\bar{\cdot})$	quantities at steady state

Problem Statement and Preliminaries

Modifier Adaptation

Consider a static plant optimization problem given by

$$\left(\bar{x}_p^{\star},\ \bar{u}_p^{\star},\ \bar{y}_p^{\star}\right) = \arg\min_{\bar{x},\bar{u},\bar{y}}\ \ell(\bar{y},\bar{u}) \tag{1a}$$

subject to

$$\bar{x} = f_p(\bar{x},\bar{u}), \tag{1b}$$

$$\bar{y} = h_p(\bar{x}), \tag{1c}$$

$$0 \geq g(\bar{y},\bar{u}), \tag{1d}$$

where $f_p : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$, $h_p : \mathbb{R}^{n_x} \to \mathbb{R}^{n_y}$ and $g : \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_g}$ and the subscript $(\cdot)_p$ is used to denote plant quantities/variables. Here we assume knowledge of the constraint function g, while the plant model (f_p, h_p) and specifically the steady-state map $u \mapsto y_p$ are essentially never known precisely. Note that limiting the uncertainty to the plants input-output behavior is without significant loss of generality, cf.[44] Hence, at each RTO iteration j the modifier adaptation approach is built upon solving the modified model optimization problem

$$(\bar{x}_j,\ \bar{u}_j,\ \bar{y}_j) = \arg\min_{\bar{x},\bar{u},\bar{y}} \ell(\bar{y},\bar{u}) \tag{2a}$$

subject to

$$\bar{x} = f(\bar{x},\bar{u}), \tag{2b}$$

$$\bar{y} = h(\bar{x}) + \varepsilon_{j-1} + \Lambda_{j-1}(\bar{u} - \bar{u}_{j-1}), \tag{2c}$$

$$0 \geq g(\bar{y},\bar{u}), \tag{2d}$$

wherein the usual first-order corrections are employed, cf.[5,6] The (output) modifiers $\varepsilon \in \mathbb{R}^{n_y}$ and $\Lambda \in \mathbb{R}^{n_y} \times \mathbb{R}^{n_u}$ are defined using

$$\begin{aligned}\tilde{\varepsilon}_j &= \quad H_p(\bar{u}_j) - \quad H(\bar{u}_j),\\ \tilde{\Lambda}_j &= \mathrm{D}H_p(\bar{u}_j) - \mathrm{D}H(\bar{u}_j),\end{aligned}$$

and a filtering step, i.e.

$$\xi_{j+1} = \xi_j + \sigma(\tilde{\xi}_j - \xi_j), \quad \xi \in \{\varepsilon,\ \Lambda\},\ \sigma \in (0, 1]. \tag{3}$$

The filter is employed to avoid oscillations and to improve convergence properties.[6] In the definition of ε and Λ the matrices $H_p(\bar{u}_j)$ and $H(\bar{u}_j)$ are the steady-state input-output maps of plant, respectively, the modified model. In other words, $H_p : \mathbb{R}^{n_u} \to \mathbb{R}^{n_y}$ is the plant steady-state input-to-output map $\bar{u} \mapsto y_p = H_p(\bar{u})$, i.e. the solution of

$$\bar{x}_p = f_p(\bar{x}_p, \bar{u}), \quad \bar{y}_p = h_p(\bar{x}_p),$$

and $\mathrm{D}H_p : \mathbb{R}^{n_u} \to \mathbb{R}^{n_y \times n_u}$ is its Jacobian. Likewise $H : \mathbb{R}^{n_u} \to \mathbb{R}^{n_y}$ is the steady-state input-to-output map $\bar{u} \mapsto \bar{y} = H(\bar{u})$ of the nominal model, i.e. the solution of

$$\bar{x} = f(\bar{x}, \bar{u}), \quad \bar{y} = h(\bar{x}),$$

and $\mathrm{D}H : \mathbb{R}^{n_u} \to \mathbb{R}^{n_y \times n_u}$ is its Jacobian.

Under suitable technical conditions—availability of exact plant gradients, linear independence constraint qualifications for (1), uniqueness of the maps $\bar{u} \mapsto \bar{y}_{p,j} = H_p(\bar{u}_j)$ and $\bar{u} \mapsto \bar{y}_j = H(\bar{u}_j)$—it can be shown that upon convergence

$$\lim_{j\to\infty} \bar{y}_{p,j} = \bar{y}_p^\star \quad \text{and} \quad \lim_{j\to\infty} \bar{u}_j = \bar{u}_p^\star,$$

see[5,44] for details. We remark that sufficient convergence conditions for MA are also available, see.[6,10,45,46]

Dissipativity, Turnpikes and Nominal Economic MPC

Recent years saw tremendous progress on MPC with (almost) generic cost functions, which is commonly labeled *economic* MPC. We recall the nominal setting, i.e. assuming temporarily the availbility perfect plant models. Moreover, we focus on a branch of EMPC whose analysis relies on dissipativity properties of the underlying Optimal Control Problems (OCPs). We refer to[29,47] for recent overviews.

Economic and non-economic MPC is based on finite-horizon OCPs of the form

$$\min_{\boldsymbol{x},\boldsymbol{u}} \quad \sum_{i=0}^{N-1} \ell(y_i,u_i) + V_f(x_N) \tag{4a}$$

subject to

$$x_0 = \hat{x}_k, \tag{4b}$$

$$x_{i+1} = f(x_i,u_i), \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{4c}$$

$$y_i = h(x_i), \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{4d}$$

$$0 \geq g(y_i,u_i), \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{4e}$$

$$x_N \in \mathbb{X}_f. \tag{4f}$$

For the sake of simplicity, we assume that the problem data is sufficiently smooth and that optimal solutions—denoted as $(\boldsymbol{x}^\star, \boldsymbol{u}^\star)$—exist. Moreover, whenever convenient, we will use the following compact notation of the feasible set of OCP (4)

$$\mathbb{Z} := \left\{(x,u) \in \mathbb{R}^{n_x+n_u} \mid g(h(x),u) \leq 0\right\}.$$

Finally, we remark that $\hat{x}_k$ refers to the estimate of plant state at time k.

Turnpike and dissipativity properties of OCPs

While in tracking formulations of NMPC one commonly assumes that

$$\ell(y,u) = \ell(h(x),u) \geq \alpha(\|x-\bar{x}\|), \qquad \alpha \in \mathcal{K}_\infty,$$

i.e. the stage cost ℓ is assumed to be lower bounded by a class $\mathcal{K}_\infty$ of the distance to the desired setpoint $\bar{x}$.[1] In economic NMPC one relaxes this condition. Many stability results for EMPC require that there exists a so-called *storage function* $S : \mathbb{R}^{n_x} \to \mathbb{R}^+$ satisfying the following strict dissipation inequality

$$S(f(x,u)) - S(x) \leq -\alpha(\|(x,u)-(\bar{x},\bar{u})\|) + \ell(h(x),u) - \ell(h(\bar{x}),\bar{u}), \tag{5}$$

for all $(x,u) \in \mathbb{Z}$, where α is of class $\mathcal{K}$, see[29,30,48,49]. Observe that on the right hand side of (5) the setpoint $(\bar{x},\bar{u})$ appears. It is easy to verify that whenever (5) holds, the setpoint $(\bar{x},\bar{u})$ is the unique globally optimal equilibrium with respect to the stage cost ℓ and the constraints $\mathbb{Z}$.

Moreover, the dissipation inequality (5) implies that the underlying system $x_{i+1} = f(x_i,u_i)$ is optimally operated at the steady state $(\bar{x},\bar{u})$; i.e. for all feasible pairs $(\boldsymbol{x},\boldsymbol{u})$

$$\ell(h(\bar{x}),\bar{u}) \;\leq\; \liminf_{N\to\infty} \frac{1}{N}\sum_{i=0}^{N-1} \ell(h(x_i)),u_i).$$

We refer to[48,50] for details on the sufficiency and necessity of dissipativity.

In the context of this paper, it is worth to be remarked that optimal operation at steady state is quite common in chemical processes. Implicitly it constitutes the motivation for the hierarchical approach to combine RTO and MPC sketched in Figure 1.[2]

[1] A function $\alpha : \mathbb{R}_0^+ \to \mathbb{R}_0^+$ is said to be of class $\mathcal{K}$ if it is increasing strictly monotonous and $\alpha(0)=0$. It is said to be of class $\mathcal{K}_\infty$ if, additionally $\lim_{s\to\infty} \alpha(s) = \infty$ holds.

[2] There exist processes which are not optimally operated ate steady state, either due to intrinsic properties of the dynamics[51] or due to time-varying {disturbances, dynamics, constraints}.[52] However, whenever a process is not optimally operated at steady state it stands to reason whether or not one should apply the

Furthermore, the dissipativity property of OCP (4) is of importance as (combined with a reachability condition) it implies the existence of a turnpike property, see.[29,43,49,53] Moreover, we refer to[43,54] for results showing that turnpike and dissipativity properties of OCPs are almost equivalent. Simply put, a turnpike property of an OCP implies that for different initial conditions and different horizon lengths, the time that the optimal solution spend outside of an ε-neighborhood of the optimal steady state $(\bar{x}, \bar{u})$ is bounded independent of the horizon length, which can be also phrased as the following conceptual definition: OCP (4) is said to have a turnpike at $(\bar{x}, \bar{u})$, if for all horizon $N \in \mathbb{N}$, all $x_0 \in \mathbb{X}_0$ and all $\varepsilon > 0$

$$\Big[\text{time optimal pairs } (\boldsymbol{x}^\star, \boldsymbol{u}^\star) \text{ spent outside of } \varepsilon\text{-neighborhood of } (\bar{x}, \bar{u})\Big] \leq C(\varepsilon) < \infty.$$

For mathematically precise definitions of the turnpike properties we refer to.[43,54]

Under suitable differentiability assumptions the Necessary Conditions of Optimality (NCO) of OCP (4) are given by

$$\begin{aligned}
x_{i+1} &= f(x_i, u_i), && i \in \mathbb{I}_{[0,N-1]}, && \text{(6a)}\\
\lambda_i &= \frac{\partial}{\partial x}\left[\lambda_{i+1}^\top f(x_i, u_i) + \ell(h(x_i), u_i) + \mu_i^\top g(h(x_i), u_i)\right], && i \in \mathbb{I}_{[0,N-1]}, && \text{(6b)}\\
0 &= \frac{\partial}{\partial u}\left[\ell(h(x_i), u_i) + \lambda_{i+1}^\top (f(x_i, u_i) - x_{i+1}) + \mu_i^\top g(h(x_i), u_i)\right], && i \in \mathbb{I}_{[0,N-1]}, && \text{(6c)}\\
\mu_i &\geq 0, && i \in \mathbb{I}_{[0,N-1]}, && \text{(6d)}
\end{aligned}$$

and the boundary conditions are

$$x_0 = \hat{x}_k \quad \text{and} \quad \lambda_N = \left.\frac{\partial V_f}{\partial x}\right|_{x=x_N}. \tag{6e}$$

We refer to the NCOs above as the discrete-time Euler-Lagrange equations. It is easy to verify that (under suitable technical assumptions) any steady state of (6) is also a KKT point of the nominal model steady-state optimization problem (2a)—with $\varepsilon_j = 0$ and $\Lambda_j = 0$. In other

hierarchical approach to combine RTO and MPC sketched in Figure 1.

words, steady-state turnpikes occur only at equilibria of the Euler-Lagrange equations.[34,42,55]

Notably, *turnpikes are a property of parametric* OCP*s*, hence their importance in the analysis of (economic) MPC schemes is not surprising.[29,42,49,56] Moreover, it deserves to be said that the term *turnpike* was coined in 1958 in economics in a book of Dorfman, Solow and Samuelson.[57,58] The turnpike phenomenon has been observed already by John von Neumann in the 1930s.[59] See also[60] and[55,61] for more recent investigations.

Illustrative turnpike example. Throughout this paper we consider an isothermal Continuous-Stirred Tank Reactor (CSTR) in which two consecutive reactions occur $\mathrm{A} \xrightarrow{k_1} \mathrm{B} \xrightarrow{k_2} \mathrm{C}$. The system is subject to the following continuous-time dynamics:

$$\begin{aligned} \dot{x}_1 &= \frac{u}{V}(c_{A0} - x_1) - k_1 x_1, \\ \dot{x}_2 &= \frac{u}{V}(-x_2) + k_1 x_1 - k_2 x_2, \end{aligned} \tag{7}$$

in which x_1 and x_2 are the molar concentrations of A and B in the reactor, respectively; k_1 and k_2 are the two kinetic constants; u is the feed flow-rate (which is the manipulated input, and is assumed equal to the outlet flow-rate); V is the (constant) reactor volume; c_{A0} is the inlet concentration of A. We assume that both states (x_1, x_2) are measurable. The system parameters for the true plant are as follows:

$$k_1 = 1.0 \text{ min}^{-1}, \quad k_2 = 0.05 \text{ min}^{-1}, \quad c_{A0} = 1.0 \text{ kmol/m}^3, \quad V = 1.0 \text{ m}^3. \tag{8}$$

The cost function ℓ represents the economics of the system (expenditure for raw material - revenue from product):

$$\ell(h(x), u) = \alpha u c_{A0} - \beta u x_2, \tag{9}$$

in which $\alpha = 1.0$ €/kmol and $\beta = 4.0$ €/kmol are the prices of reactant and product, respectively. State and input constraints are given by

$$0 \leq x_1 \leq 1\,\mathrm{kmol/m^3},\ 0 \leq x_2 \leq 1\,\mathrm{kmol/m^3},\ 0 \leq u \leq 2\,\mathrm{m^3/min}. \tag{10}$$

The optimal steady state of the plant reads

$$\bar{u} = 1.04298,\ \bar{x} = \begin{bmatrix} 0.51052 & 0.46709 \end{bmatrix}^\top,\ \bar{\lambda} = \begin{bmatrix} -1.8684 & -3.8170 \end{bmatrix}^\top,\ \ell(\bar{x}, \bar{u}) = -0.90568,$$

whereby $\bar{\lambda}$ is the Lagrange multiplier corresponding to the dynamics at steady-state.

We consider the open-loop OCP (4) without any terminal constraint or penalty (i.e. $\mathbb{X}_f = \mathbb{X}$ and $V_f(x) = 0$). Without considering any plant-model mismatch we solve the open-loop OCP for different horizon lengths $N \in \{4, 8, 20, 40\}$ which considering the sampling time $h = 0.25$ min corresponds to $T \in \{1, 2, 5, 10\}$min. The initial conditions, corresponding to the different horizons, are $x_0 \in \{[0.3, 0.3]^\top,\ [0.75, 0.75]^\top,\ [0.3, 0.3]^\top,\ [0.75, 0.75]^\top\}$.

The results are obtained using a direct multiple shooting implemented in CasADi,[62] in which the system and cost are discretized using the backward Euler scheme, as detailed. Given a sampling time h, the system (7) and the cost (9), this yields

$$\begin{aligned} x_1^+ &= \frac{x_1 + \frac{u}{V} c_{A0} h}{1 + k_1 h + \frac{u}{V} h}, \\ x_2^+ &= \frac{x_2 + k_1 h \left(\frac{x_1 + \frac{u}{V} c_{A0} h}{1 + k_1 h + \frac{u}{V} h} \right)}{1 + k_2 h + \frac{u}{V} h}, \end{aligned} \tag{11}$$

$$\ell(x, u) = (\alpha u c_{A0} - \beta u x_2^+) h. \tag{12}$$

The results are shown in Figure 2. As one can see in the top three plots that with increasing horizon length N the state and inputs approach a neighborhood of their optimal steady-state values (dotted green). The quintessence of the turnpike property is that the longer the horizon is the more time is spend close to the optimal steady state (aka the turn-

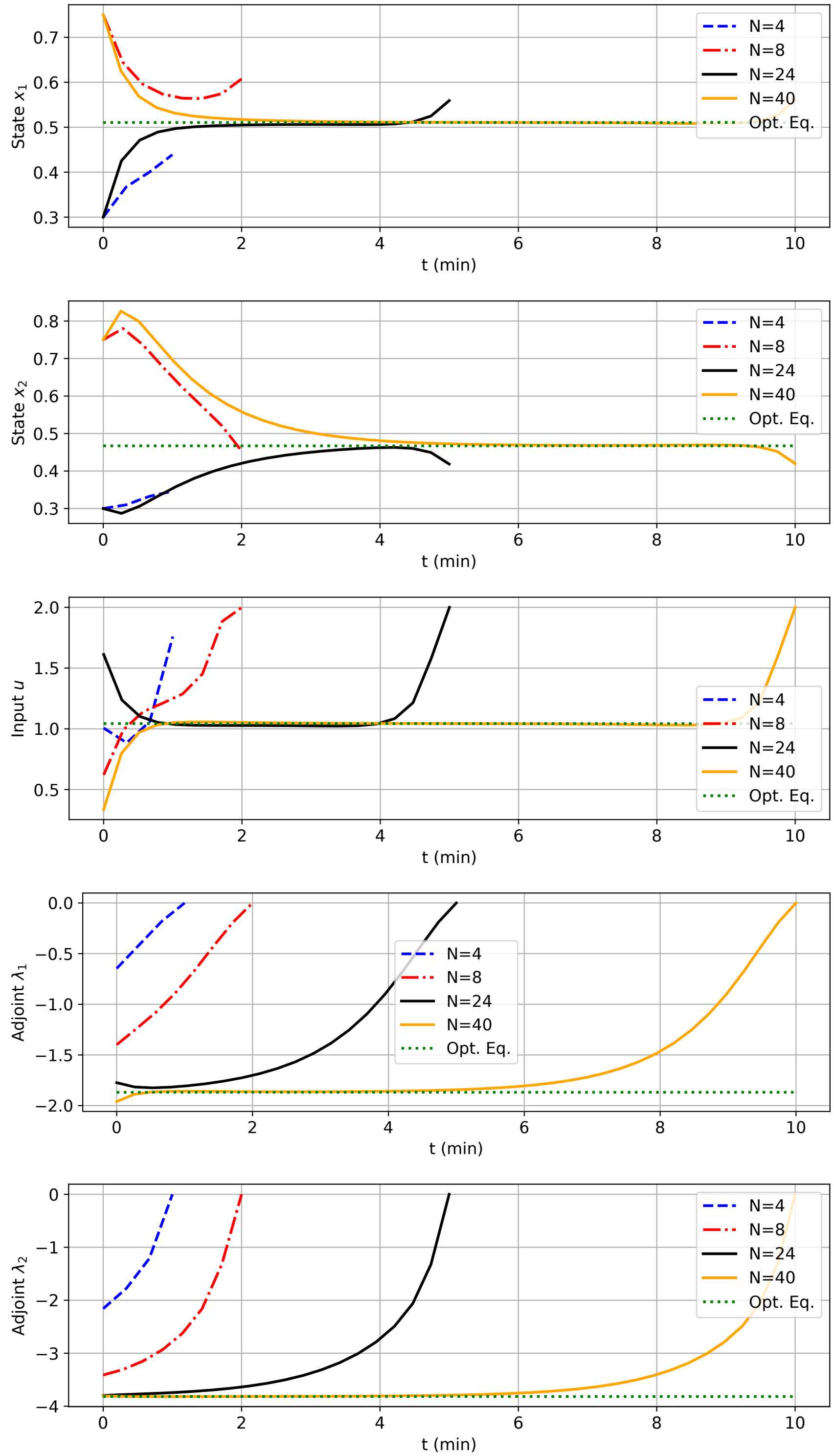

Figure 2: Comparative open-loop results considering $\mathbb{X}_f = \mathbb{X}$ and $V_f(x) = 0$ for $N \in \{4, 8, 20, 40\}$ ($T \in \{1, 2, 5, 10\}$min) and different initial conditions: states (top two), input (middle) and adjoints (bottom two).

pike). Moreover, the adjoints—i.e. the multipliers corresponding to the equality constraints stemming from the discretized dynamics—also approach the values corresponding to the optimal steady state. This is in line with the continous-time results of Trelat and Zuazua[55] or with.[42] Eventually, as the open-loop OCP does not entail any terminal constraint or penalty, the adjoints obey the terminal condition

$$\lambda_N = 0,$$

cf. (6) and see[42,63] for a detailed discussion.

Stability of nominal EMPC

Coming back to nominal EMPC based on OCP (4), it is apparent that there are three main ingredients for stability:

- the terminal penalty $V_f : \mathbb{R}^{n_x} \to \mathbb{R}$;
- the terminal constraint set $\mathbb{X}_f \subseteq \mathbb{R}^{n_x}$; and
- the horizon length $N \in \mathbb{N}$.

In the context of dissipativity-based results on stability of EMPC one can distinguish three main approaches as summarized in Table 2.[3]

The results in[30,48] use $\mathbb{X}_f = \bar{x}$ and $V_f(x_N) = 0$—while the horizon N is chosen such that OCP (4) is feasible—to show under suitable technical conditions (dissipativity and continuity of the optimal value function) asymptotic stability of $\bar{x}$, cf. for example Theorem 3.2 and Corollary 3.3 in.[29] This approach can also be generalized to terminal sets.[64]

Moreover, in[31,49,65,66] it is shown that, for sufficiently large N, the choice $\mathbb{X}_f = \mathbb{R}^{n_x}$ and $V_f(x_N) = 0$ leads to practical asymptotic stability of $\bar{x}$, whereby the size of the attractive neighborhood of $\bar{x}$ depends on the horizon length. Core assumptions are dissipativity and

[3]There also exist analysis results that do not require dissipativity, see[29,47] for recent overviews.

Table 2: Overview of dissipativity-based stability conditions for nominal economic NMPC.

V_f	$\mathbb{X}_f$	N	Closed Loop Prop.	References
0	$\bar{x}$	chosen for feasibility of OCP (4)	asympt. stable	[30,48]
0	$\mathbb{R}^{n_x}$	sufficiently long	prac. asympt. stable	[49,61,66]
$\bar{\lambda}^\top x_N$	$\mathbb{R}^{n_x}$	sufficiently long	asympt. stable	[34,42]

exponential reachability of $\bar{x}$, cf. for example Theorem 4.1 in.[29] Recursive feasibility can be shown under mild assumptions.[29,66]

Finally, the recent papers[34,42] propose $\mathbb{X}_f = \mathbb{R}^{n_x}$ and $V_f(x_N) = \bar{\lambda}^\top x_N$, where $\bar{\lambda}$ is the Lagrange multiplier corresponding of the stationary dynamics $x = f(x, u)$ corresponding to the optimal steady-state $(\bar{x}, \bar{u})$. Assuming dissipativity and exponential reachability of $\bar{x}$ (and technical regularity conditions) it is shown that, for sufficiently large horizon N, the optimal steady state $\bar{x}$ will be asymptotically stable. In essence this approach combines ideas on the local rotation of the stage cost ℓ from[67,68] with the turnpike approach from.[49,66] Actually, the linear end penalty $V_f(x_N) = \bar{\lambda}^\top x_N$ has two interpretations. From the primal point of view it is a correction of the gradient of ℓ at steady state, while from the dual/adjoint point of view it imposes a terminal condition on the adjoints of the OCP (4). We refer to[34,42] for an in-depth discussion.

Illustrative turnpike example revisited. To illustrate the effect of the linear end penalty $V_f(x_N) = \bar{\lambda}^\top x_N$ on the open-loop predictions, we revisit the CSTR example. Similar to before we solve the open-loop OCP for different horizon lengths $N \in \{4, 8, 20, 40\}$ which considering the sampling time $h = 0.25$ min corresponds to $T \in \{1, 2, 5, 10\}$min. The initial conditions are as before $x_0 \in \{[0.3, 0.3]^\top, [0.75, 0.75]^\top, [0.3, 0.3]^\top, [0.75, 0.75]^\top\}$. While Figure 2 shows open-loop optimal solutions for $V_f(x_N) = 0$, Figure 3 depicts open-loop predictions for $V_f(x_N) = \bar{\lambda}^\top x_N$, where $\bar{\lambda}$ is Lagrange mutliplier corresponding to the optimal steady state $(\bar{x}, \bar{u})$.

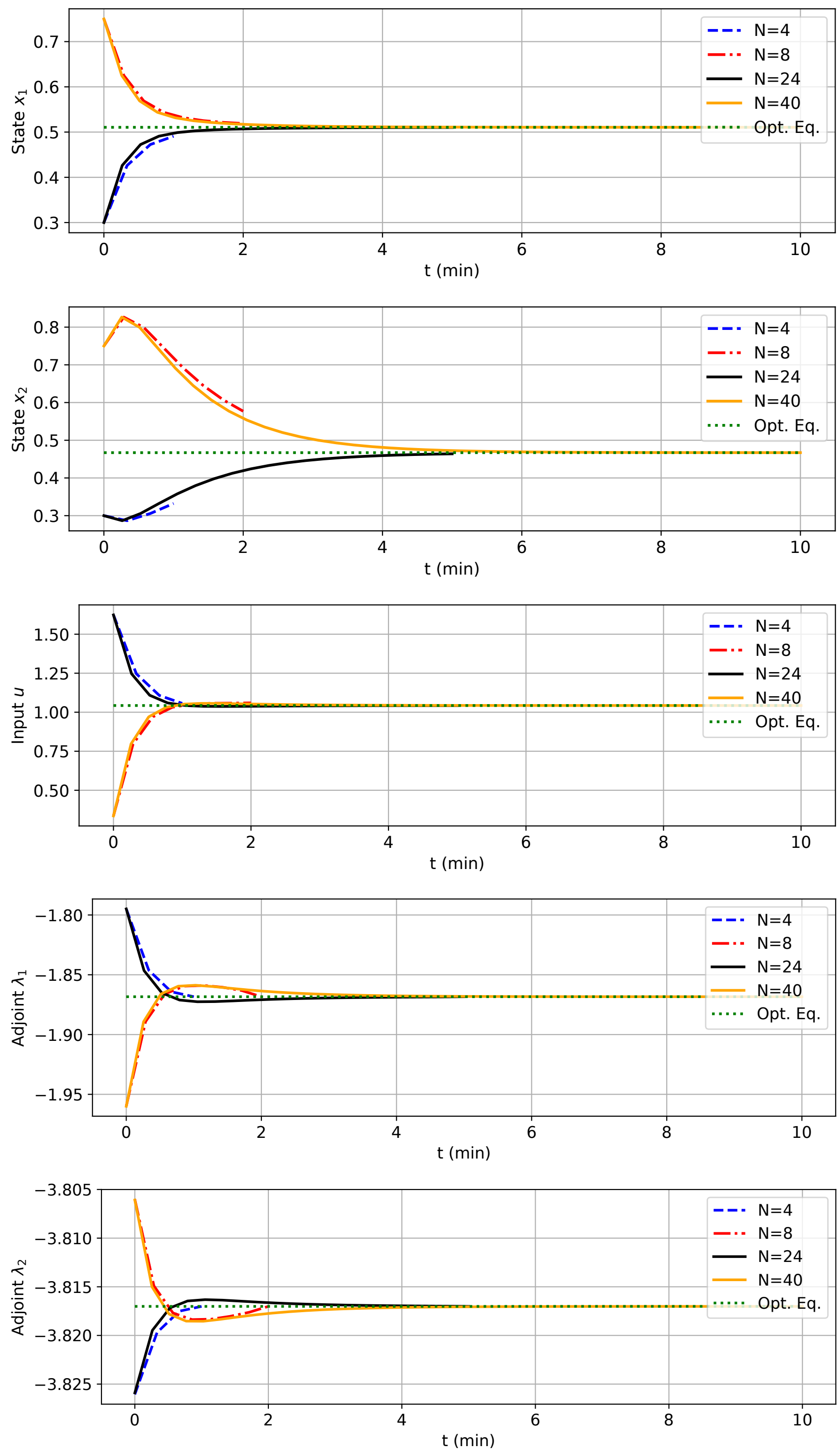

Figure 3: Comparative open-loop results for $N \in \{4, 8, 20, 40\}$ ($T \in \{1, 2, 5, 10\}$min), $V_f(x_N) = \bar{\lambda}^\top x_N$ and different initial conditions: states (top two), input (middle) and adjoints (bottom two).

Observe that, in contrast to Figure 2, in Figure 3 towards the end of the horizon states and input do not leave their turnpike values. Moreover, also note that the adjoints converge to their optimal steady-state values. As shown in[34,42] it is this difference between Figure 2 and Figure 3—or equivalently between OCP (4) with $V_f(x_N) = 0$ and with $V_f(x_N) = \bar{\lambda}^\top x_N$—which modulo technical assumptions leads to the difference between practical asymptotic stability and asymptotic stability of the closed EMPC loop.

Offset-free EMPC with Terminal Constraints

We now address the case in which there is mismatch between the model (f, h) and the actual plant (f_p, h_p). Depending on the extent of such model error, it is possible that closed-loop stability properties are lost, but even if stability still holds, the closed-loop system may not converge to the true plant optimal equilibrium $\left(\bar{y}_p^\star,\ \bar{u}_p^\star\right)$.

The same situation is typically faced and addressed in offset-free TMPC algorithms by augmenting the nominal model with additional states having integral dynamics, and estimating them along with the model states from plant outputs. Such formulations ensure that, if the closed-loop convergences to an equilibrium, then the output tracks a given output setpoint.[69] Recent formulations of offset-free MPC have been developed to achieve the same goal in the context of economic MPC by merging the approach of offset-free tracking MPC with Modifier Adaptation RTO.[39,40] In particular, the goal of such formulations here reviewed is that if the closed-loop system reaches an equilibrium, this corresponds to the most profitable equilibrium for the actual plant. Such a controller, name *offset-free economic* MPC, is composed by three main modules, as depicted in Figure 4:

(i) an augmented state and disturbance observer;

(ii) a modifier-adaptation target optimizer; and

(iii) a modifier-adaptation optimal control problem solver.

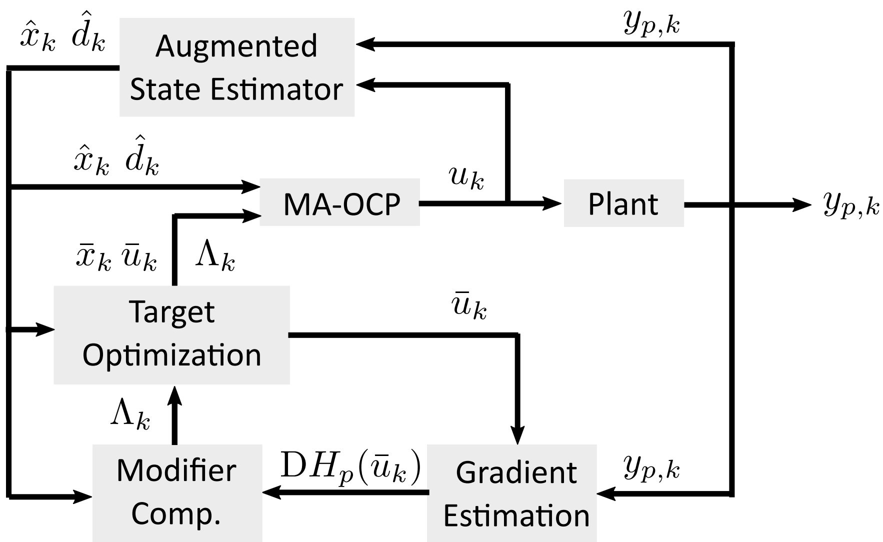

Figure 4: Block diagram of offset-free EMPC with terminal constraints.

State and disturbance observer. Given the nominal model functions, (f, h), an augmented system is defined in order to obtain, asymptotically, zero prediction error despite plant/model mismatch. Among the many different available disturbance models and observers[69], we consider the following augmented prediction model:

$$
\begin{aligned}
x_{k+1} &= f(x_k, u_k) + B_d d_k, \\
d_{k+1} &= d_k, \\
y_k &= h(x_k) + C_d d_k,
\end{aligned}
\tag{13}
$$

in which $d \in \mathbb{R}^{n_y}$ is usually referred to as disturbance, and the matrices $B_d \in \mathbb{R}^{n_x \times n_y}$ and $C_d \in \mathbb{R}^{n_y \times n_y}$ can be chosen by the designer to model the effect of such disturbance on the state and output maps.

Given the plant output measurement at time k, denoted by $y_{p,k}$ and the corresponding output predicted by the augmented model (13), denoted by y_k, we define the prediction error as

$$
e_k = y_{p,k} - y_k. \tag{14}
$$

Given the state and disturbance predictions obtained from the augmented model (13), denoted by (x_k, d_k), we compute the corresponding estimates as

$$\begin{aligned} \hat{x}_k &= x_k + K_x e_k, \\ \hat{d}_k &= d_k + K_d e_k, \end{aligned} \tag{15}$$

in which the matrices $K_x \in \mathbb{R}^{n_x \times n_y}$ and $K_d \in \mathbb{R}^{n_y \times n_y}$ are chosen to form a (nominally) asymptotically stable observer. This implies, in particular, that K_d is invertible.[70]

We note that in the special case of state feedback, i.e. $h_p(x) = h(x) = x$, a state disturbance model can be used by choosing $B_d = I$ and $C_d = 0$ coupled with a deadbeat observer $K_x = I$ and $K_d = I$. This leads to the following deadbeat filtered state and disturbance:

$$\begin{aligned} \hat{x}_k &= x_k + (x_{p,k} - x_k) = x_{p,k}, \\ \hat{d}_k &= d_k + (x_{p,k} - x_k) = x_{p,k} - f(\hat{x}_{k-1}, u_{k-1}). \end{aligned} \tag{16}$$

Hence, it follows that the model state is realigned to the true plant state, and the disturbance is equal to the so-called innovation $x_{p,k} - f(\hat{x}_{k-1}, u_{k-1})$.

Steady-state target optimization with modifier adaptation. A target calculation is needed at each sampling time to compute the equilibrium $(\bar{x}_k,\ \bar{u}_k,\ \bar{y}_k)$ given that the disturbance estimate $\hat{d}_k$ changes if $e_k \neq 0$. In tracking MPC, this equilibrium pair is computed so that the augmented model steady-state output is equal to the given setpoint. In economic MPC instead we compute the equilibrium so-that the equilibrium cost function $\ell(\bar{y}_k, \bar{u}_k)$ is minimized. However, in order for this equilibrium to converge to the true optimal equilibrium, we need to add a first-order modifier as in (2c).

Thus, the target problem to be solved at time k is:

$$(\bar{x}_k,\ \bar{u}_k,\ \bar{y}_k) = \underset{(x,u,y)}{\arg\min}\, \ell(y,u) \tag{17a}$$

subject to

$$x = f(x,u) + B_d \hat{d}_k, \tag{17b}$$

$$y = h(x) + C_d \hat{d}_k + \Lambda_k (u - \bar{u}_{k-1}), \tag{17c}$$

$$0 \geq g(y,u), \tag{17d}$$

in which $\Lambda_k \in \mathbb{R}^{n_y \times n_u}$ is the current modifier matrix, later defined. The modifier matrix is initialized as $\Lambda_0 = 0$, and updated at each decision time as follows:

$$\Lambda_{k+1} = (1-\sigma)\Lambda_k + \sigma \left(\mathrm{D}H_p(\bar{u}_k) - \mathrm{D}H(\bar{u}_k, \hat{d}_k) \right), \tag{18}$$

in which $H : \mathbb{R}^{n_u \times n_y} \to \mathbb{R}^{n_y}$ is the augmented model steady-state input-to-output map $\bar{u} \mapsto \bar{y} = H(\bar{u}, \hat{d}_k)$, i.e. the solution of

$$\bar{x} = f(\bar{x}, \bar{u}) + B_d \hat{d}_k, \qquad \bar{y} = h(\bar{x}) + C_d \hat{d}_k,$$

and $\mathrm{D}H : \mathbb{R}^{n_u \times n_y} \to \mathbb{R}^{n_y \times n_u}$ is its Jacobian with respect to $\bar{u}$.

Remark 1 (RTO and MPC sampling rates)**.** *It is important to remark that, for simplicity of presentation, we are assuming that the plant Jacobian update occurs at the same rate as the three offset-free* MPC *modules (observer, target calculation, and* OCP*), and hence we are not explicitly distinguishing between* RTO *(i.e. plant gradient estimation) index j and* MPC *index k. In general, it is possible that in* (18) *the plant Jacobian $\mathrm{D}H_p(\cdot)$ is updated at a different (obviously lower) rate. However, note that even in this case, as the offset correction $C_d \hat{d}_k$ in* (17c) *is updated at each time step k, one still needs to resolve the target problem at each* *time-step k. Moreover, the modifier update* (18) *also runs at time index k and would read*

$$\Lambda_{k+1} = (1-\sigma)\Lambda_k + \sigma\left(\mathrm{D}H_p(\bar{u}_j) - \mathrm{D}H(\bar{u}_k, \hat{d}_k)\right).$$

Remark 2 (Relation to Modifier Adaptation)**.** *We remark that the estimation of the disturbance $\hat{d}_k$—and especially the underlying deadbeat observer—bear substantial similarity to constraint adaptation, which is a specific variant of* MA *relying on zeroth-order corrections, see.*[41] *Moreover, the recent approach to using transient measurements in constraint adaptation*[71] *is closely related to a deadbeat observer.*

We also notice that, compared to (2a)*, the zero-order term ε is not present in* (17c) *given that its role is replaced by the disturbance estimate $\hat{d}_k$. Furthermore, notice that if we set $B_d = 0$, $C_d = I$, $K_x = 0$ and $K_d = I$, the target optimization problem* (17) *is equivalent to the ouptut modifier-adaption* RTO *problem* (2a)*.*

OCP with modifier adaptation. As last module, the OCP solved at each decision time is here described, which takes into account the augmented system dynamics and it embeds a steady-state modifier, as in the target optimization (17), to ensure convergence towards the target, and hence towards to the true plant equilibrium. Given the current state and

Initialize $\hat{d}_0 = 0$, $\Lambda_0 = 0$, $\bar{u}_0 = 0$;
while do
  Get measurement $y_{p,k}$;
  Compute state, disturbance and output predictions from (13);
  Solve the target optimization problem (17) to obtain state, input targets $(\bar{x}_k, \bar{u}_k)$;
  Solve the OCP (19) to obtain optimal solution $(\boldsymbol{x}^\star, \boldsymbol{u}^\star)$;
  Apply feedback $u_k = u_0^\star(\hat{x}_k)$ to plant;
  Get plant gradient information $\mathrm{D}H_p(\bar{u}_k)$;
  Update modifier matrix Λ_{k+1} (18);
  Update time index $k \leftarrow k+1$;
end

Algorithm 1: Offset-free EMPC with terminal constraints.

disturbance estimates $(\hat{x}_k, \hat{d}_k)$ and the current input target $\bar{u}_k$, we solve the following OCP:

$$\min_{\boldsymbol{x},\boldsymbol{u}} \sum_{i=0}^{N-1} \ell(y_i, u_i) \tag{19a}$$

subject to

$$x_0 = \hat{x}_k, \tag{19b}$$

$$x_{i+1} = f(x_i, u_i) + B_d \hat{d}_k, \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{19c}$$

$$y_i = h(x_i) + C_d \hat{d}_k + \Lambda_k (u_i - \bar{u}_k), \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{19d}$$

$$0 \geq g(y_i, u_i), \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{19e}$$

$$x_N = \bar{x}_k. \tag{19f}$$

Denoting the optimal solution of this problem as $(\boldsymbol{x}^\star, \boldsymbol{u}^\star)$, the first input of the optimal sequence is actually implemented in closed loop, according to the usual receding horizon principle, i.e.

$$u_k = u_0^\star(\hat{x}_k). \tag{20}$$

The offset-free EMPC is summarized in Algorithm 1.

We can state the main properties of this offset-free economic EMPC, which can be proved by KKT matching techniques as in[5,6,38], taking into account the fact that the prediction errors goes to zero[39] and the convergence properties of EMPC with terminal constraint[30].

Conjecture 1 (Optimality properties)**.**
Assume that problems (17) *and* (19) *remain feasible at all times, and that the closed-loop system:*

$$\begin{aligned} x_{p,k+1} &= f_p(x_{p,k}, u_k), \\ y_{p,k} &= h_p(x_{p,k}), \end{aligned} \tag{21}$$

with u_k given in (20) *reaches an equilibrium with input and output:*

$$\lim_{k\to\infty} u_k = u_\infty, \quad \lim_{k\to\infty} y_{p,k} = y_{p,\infty}.$$

It follows that the reached equilibrium is the optimal one for the plant, i.e.:

$$y_{p,\infty} = \lim_{k\to\infty} \bar{y}_k = \bar{y}_p^\star, \qquad u_\infty = \lim_{k\to\infty} \bar{u}_k = \bar{u}_p^\star. \tag{22}$$

Remark 3 (Estimation of plant gradients)**.** *We observe that a crucial step in Algorithm 1 is the estimation of steady-state input-output plant Jacobian, $\mathrm{D}H_p(\bar{u}_k)$, which can be done in difference ways,[6] e.g. by using finite-difference approximations, Broyden's methods, fitted surfaces, or dynamic (linear) systems identification.[39] In the sake of simplicity this (important) aspect of the considered method is not elaborated in this work, and we assume that plant gradients are available.*

Offset-free EMPC without Terminal Constraints

The previous section has already shown how one can closely integrate offset-free EMPC with modifier adaptation. However, as mentioned in Remark 1, so far the need for resolving the target optimziation problem at each time step k could not be alleviated. Next, we show how the recent progress on EMPC without terminal constraints allows doing so.

To the end of removing it from the picture, lets recapitulate the purpose of the target optimization problem (17) in Algorithm 1: it provides the steady state $(\bar{x}_k, \bar{u}_k)$ which enters the OCP (19) in the terminal constraint (19f) and in the modified output equation (19d).

However, as we have seen earlier in the paper—and especially in the results of Figure 2—the turnpike property implies that for sufficiently long horizons the open-loop predictions of states and adjoints will stay close to their optimal steady values for a substantial part of the prediction horizon. In other words, provided the open-loop predictions exhibit the turnpike phenomenon, the solution to the open-loop OCP also gives estimates/approximations of the optimal steady state $(\bar{x}_k,\ \bar{u}_k)$.

Based on this observation we suggest using the following OCP in the MPC scheme

$$\min_{\boldsymbol{x},\boldsymbol{u}} \sum_{i=0}^{N-1} \ell(y_i, u_i) + \hat{\lambda}_k^\top x_N \tag{23a}$$

subject to

$$x_0 = \hat{x}_k, \tag{23b}$$

$$x_{i+1} = f(x_i, u_i) + B_d \hat{d}_k, \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{23c}$$

$$y_i = h(x_i) + C_d \hat{d}_k + \Lambda_k (u_i - \hat{u}_k), \qquad i \in \mathbb{I}_{[0,N-1]}, \tag{23d}$$

$$0 \geq g(y_i, u_i), \qquad i \in \mathbb{I}_{[0,N-1]}. \tag{23e}$$

Observe that this OCP does not entail any terminal constraint, it does however use the gradient correcting end penalty $\hat{\lambda}_k^\top x_N$.

As usual in the MPC context, $x^\star(i|\hat{x}_{k-1})$ denotes the value of the optimal predicted state trajectory at time $i \in \mathbb{I}_{[0,N-1]}$ corresponding to the initial condition—i.e. the state estimate—$\hat{x}_{k-1}$.[4] Likewise let $u^\star(i|\hat{x}_{k-1})$ and $\lambda^\star(i|\hat{x}_{k-1})$ denote the optimal input and adjoint trajectories. Then, instead of obtaining $\hat{\lambda}_k$ and $\hat{u}_k$ by solving an explicit target optimization, we

[4]For the sake of readability we surpress here that the predicted state trajectories also depend on $\hat{d}_k$ and Λ_k.

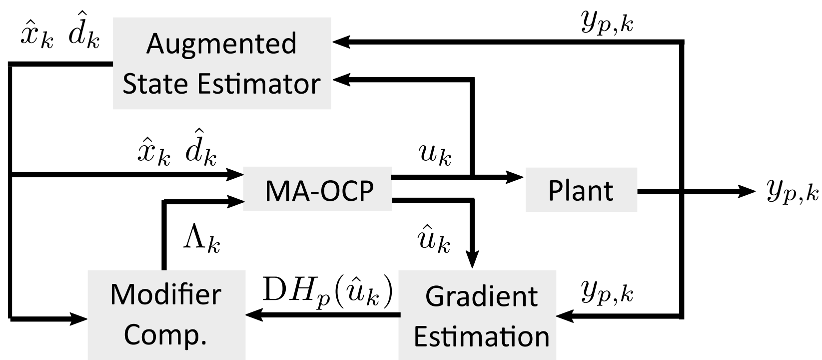

Figure 5: Block diagram of proposed scheme.

suggest using the following estimates:

$$\hat{u}_k \doteq u^\star(\tfrac{N}{2}|\hat{x}_{k-1}), \tag{24a}$$

$$\hat{\lambda}_k \doteq \lambda^\star(\tfrac{N}{2}|\hat{x}_{k-1}). \tag{24b}$$

That is, we approximate the turnpike values of inputs and adjoints by evaluating the most recent prediction in the middle of horizon at $i = \frac{N}{2}$. The choice $i = \frac{N}{2}$ is motivated by the observation that it is in the middle of optimization horizon where the open-loop predictions stay close to their turnpike values, cf. the example in Figure 2. Put differently, we exploit the turnpike property as an implicit predictor of the optimal steady state input (and the corresponding Lagrange multiplier). We remark that this combines the offset-free EMPC[38] with the results on EMPC without terminal constraints.[42] Moreover the idea to use the open-loop predictions as approximators of the optimal steady state adjoint has first been suggested in.[42]

OCP (23) leads to the blend of modifier adaptation and offset-free EMPC summarized in Algorithm 2 and in Figure 5. Observe that in the proposed scheme the modifier computation, solving the OCP and the gradient estimation take the role of the classical RTO loop, cf. also Figure 4.

Instead of providing a detailed formal analysis of the properties of Algorithm 2, we phrase a conjecture backed up by existing results from RTO and MPC.

Initialize $\hat{d}_0 = 0$, $\Lambda_0 = 0$, $\hat{u}_0 = 0$, $\hat{\lambda}_0 = 0$;
while do
  Get measurement $y_{p,k}$;
  Compute state, disturbance and output predictions from (13);
  Solve the OCP (23) to obtain optimal solution $(\boldsymbol{x}^\star, \boldsymbol{u}^\star, \boldsymbol{\lambda}^\star)$;
  Apply feedback $u_k = u_0^\star(\hat{x}_k)$ to plant;
  Get $\hat{\lambda}_{k+1}$ and $\hat{u}_{k+1}$ from $(\boldsymbol{x}^\star, \boldsymbol{u}^\star, \boldsymbol{\lambda}^\star)$ via (24);
  Get plant gradient information $\mathrm{D}H_p(\hat{u}_k)$;
  Update modifier matrix Λ_{k+1} (18);
  Update time index $k \leftarrow k+1$;
end

Algorithm 2: Offset-free economic MPC without terminal constraints.

Conjecture 2 (Stability and optimality properties)**.**

Consider Algorithm 2.

1. *Suppose that* $B_d = 0$, $C_d = I$, $K_x = 0$ *and* $K_d = I$ *in* (15).
2. *Let exact steady-state plant gradient estimates be available at each iteration* k.
3. *Let the steady-state input-output maps of plant and model* $\mathrm{D}H_p$ *and* $\mathrm{D}H$ *be real-valued functions.*[5]
4. *For all* $\hat{d}_k$ *and all* Λ_k *let the* OCP (23) *have a turnpike property with respect to* $(\bar{x}_k, \bar{u}_k, \bar{\lambda}_k)$, *whereby* $(\bar{x}_k, \bar{u}_k) \in \operatorname{int} \mathbb{Z}$.
5. *Let* OCP (23) *be feasible at all iterations* $k \in \mathbb{N}$.

Then, for sufficiently large prediction horizon N*, upon convergence one has*

$$y_{p,\infty} = \lim_{k\to\infty} \bar{y}_k = \bar{y}_p^\star, \qquad u_\infty = \lim_{k\to\infty} \bar{u}_k = \bar{u}_p^\star. \tag{25}$$

Conditions 1–3 are motivated by the fact that under the hood the proposed scheme is based on output modifier adaptation. Conditions 4–5 stem from EMPC without terminal constraints.[42] However in contrast to[42] it might be necessary to assume recursive feasibility

[5]Hence the image $\bar{y}_p = \mathrm{D}H_p(\bar{u})$ is unique for all $\bar{u}$, likewise for $\mathrm{D}H$.

as the location of the turnpike will vary as the offset estimate $\hat{d}_k$ and the modifier Λ_k change over time. Moreover, the analysis in[42] indicates that the horizon N should be sufficiently long a) to ensure that the quality of the steady-state approximation (24) and b) to foster recursive feasibility of OCP (23). A detailed analysis and the proof of the conjecture above is postponed to future work.

The role of turnpike properties in merging RTO and MPC. Observe that Algorithm 2 does not involve any target optimization problem. Instead it relies on the fact that—provided OCP (23) exhibits the turnpike property—the open-loop predictions provide approximations of the solution to the target optimization problem (17). Hence the turnpike property is crucial in ensuring that (24) provides an approximation of the (input, adjoint) values at steady state. As mentioned earlier, this is no coincidence as steady-state turnpikes are steady states of the NCO (6). A detailed analysis of the relation between the turnpike values of states, inputs and adjoints and the corresponding optimal steady state values can be found in.[34,55]

Moreover, it deserves to be noted that, whenever the open-loop predictions do not exhibit the (steady-state) turnpike phenomenon, then the underlying system is not optimally operated at steady state. In this case it might indeed be better—from the point of view of minimizing $\sum_i \ell(x_i, u_i)$—to track an optimal orbit. However, it is so far not clear how this can be incorporated into the classical hierarchy of RTO and MPC (Figure 1).

The role of RTO in merging RTO and MPC. Interestingly, while in Algorithm 1 one can still identify an explicit presence of RTO—i.e. the target optimization problem (17) takes this role and it can be shown to be equivalent to output modifier adaptation—in the merged framework of Algorithm 2 there is no explicit occurrence of any steady-state optimization. Rather the turnpike property implies that the open-loop optimal predictions provide approximate solutions to the steady-state optimization.

This observation leads to the question of *what is the remaining role of* RTO *in merging*

RTO *and* MPC*?* As already pointed out in,[72] in general, *plant gradient estimation is an important issue in* RTO. One might even say that the whole family of modifier adaptation schemes (except constraint adaptation) hinges crucially on the availability of accurate estimates of plant gradients. Likewise the performance of the proposed Algorithm 2 is expected to rely on the availability of gradient estimates. Hence in the proposed framework the active role of RTO is in providing tools and methods for estimating steady-state plant gradients from available measurement data.

Illustrative Examples

Example 1: isothermal CSTR with consecutive reactions

Steady-state plant-model mismatch analysis. We return to the illustrative CSTR example from before. We consider the available model not to match the plant, i.e. the plant considers both reactions A $\xrightarrow{k_1}$ B $\xrightarrow{k_2}$ C with $k_1 = 1.0\,\mathrm{min}^{-1},\ k_2 = 0.05\,\mathrm{min}^{-1}$, while in the model the side reaction B $\xrightarrow{k_2}$ C is neglected and an incorrect kinetic constant k_1 is used, i.e. $k_1 = 0.9\,\mathrm{min}^{-1},\ k_2 = 0.0\,\mathrm{min}^{-1}$. Observe that the steady-states $\bar{x}_1, \bar{x}_2$ can be parametrized by $\bar{u}$

$$\bar{x}_1 = \frac{\bar{u}}{Vk_1 + \bar{u}} c_{A0}, \tag{26a}$$

$$\bar{x}_2 = \frac{Vk_1}{Vk_2 + \bar{u}} \cdot \bar{x}_1 = \frac{Vk_1}{Vk_2 + \bar{u}} \cdot \frac{\bar{u}}{Vk_1 + \bar{u}} c_{A0}. \tag{26b}$$

Hence the steady-state stage cost $\ell(h(\bar{x}), \bar{u})$ can be parametrized by $\bar{u}$ as well. Figure 6 depicts the feasible steady states and the steady-state stage cost for plant and model. As one can see, there exists a considerable plant-model mismatch.

Comparative simulation study. We compare the following control strategies:

- Nominal EMPC, i.e. the MPC controller uses the inexact model (EMPC_{Nom}).

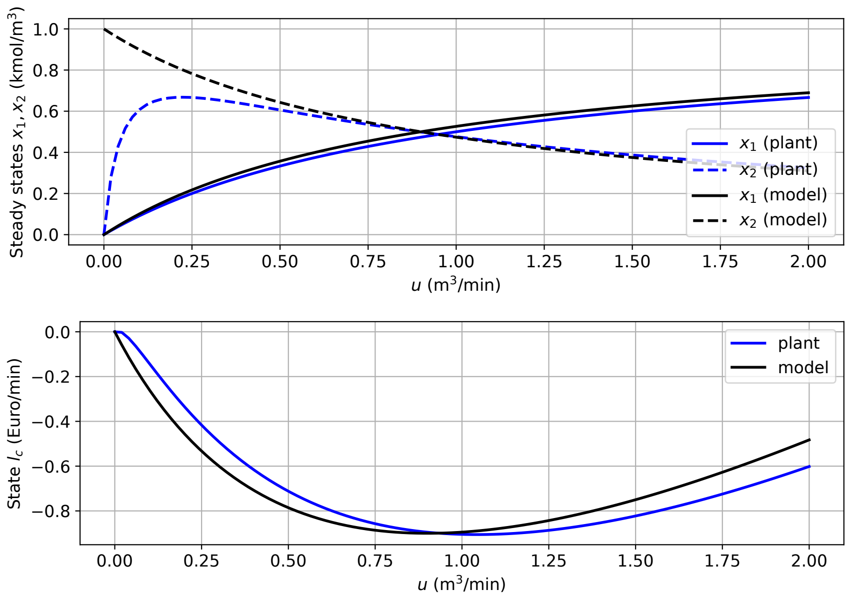

Figure 6: CSTR – Steady states for plant and model (top) and steady-state stage cost (bottom).

- Offset-free TMPC with terminal constraint (TMPC$_{MA}$).[6]
- Offset-free EMPC with terminal constraints as illustrated in Figure 4 (EMPC$_{MA}$).
- Offset-free EMPC without terminal constraints as illustrated in Figure 5 (EMPC$_{NoTerm}$).

Both plant and model are given by the discretized model (11) in which $h = 0.25$ min, but the MPC model uses incorrect parameters. For all strategies we consider a sampling period of $h = 0.25$ min and a prediction horizon of $N = 24$ which corresponds to $T = 6$ min. The simulation horizon for the closed-loop is set to $T_{sim} = 10$ min. We assume that at each sampling time k exact plant gradient information is available. For the schemes EMPC$_{MA}$ TMPC$_{MA}$, and EMPC$_{NoTerm}$ we consider the modifier update (18) to be executed at the same sampling rate as the MPC controller. Moreover, TMPC$_{MA}$, and EMPC$_{NoTerm}$ consider the filter gain $\sigma = 0.2$, while EMPC$_{MA}$ uses $\sigma = 0.075$.[7] For the sake of simplicity, all terminal

[6]In this scheme the continuous-time stage cost is $\ell(x, u) = (x - \bar{x}_k)^\top Q(x - \hat{x}_k) + (u - \bar{u}_k)^\top R(u - \hat{u}_k)$ with $Q = I$ and $R = 0.0001$.

[7]Using larger values of σ the target optimization starts to oscillate close to the plant optimum. In contrast the EMPC$_{NoTerm}$ scheme converges to the true plant optimum for all $\sigma \in (0, 1]$.

equality constraints are approximated by the end penalty $V_N(x) = 10^3 \cdot \|x - \hat{x}_k\|^2$. The initial condition is $x_{p,0} = [0, 0]^\top$.

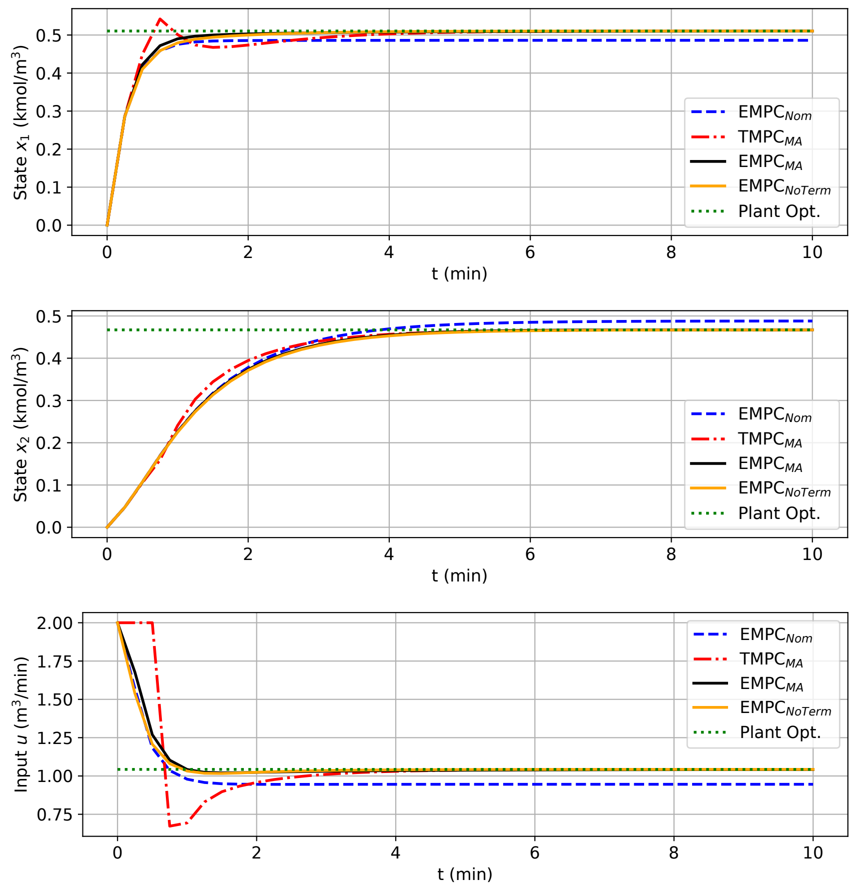

Figure 7: CSTR – Closed-loop trajectories for the control schemes EMPC$_{Nom}$, EMPC$_{MA}$, TMPC$_{MA}$, and EMPC$_{NoTerm}$.

The closed-loop trajectories are shown in Figure 7. As one can see the nominal EMPC shows the expected behavior, i.e. it does not converge to the true plant optimum, while the other three schemes do converge despite the plant-model mismatch. Note that both offset-free economic MPC schemes converge in similar fashion—although EMPC$_{MA}$ uses a small modifier filter gain of $\sigma = 0.075$, while EMPC$_{NoTerm}$ considers the gain $\sigma = 0.2$. Moreover, observe that the usual combination of TMPC with MA uses more aggressive inputs early on.

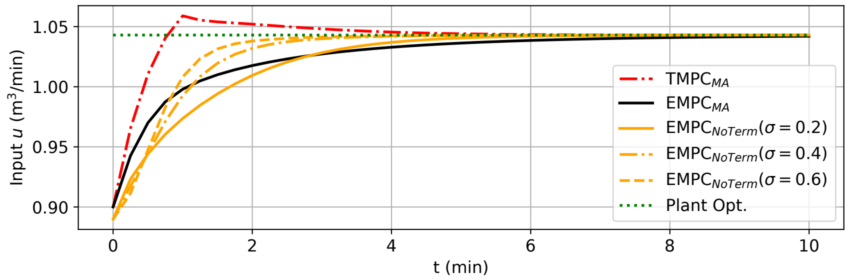

Figure 8: CSTR – Trajectories of steady-state input targets $\bar{u}_k$, respectively, $\hat{u}_k$ for the control schemes EMPC$_{MA}$, TMPC$_{MA}$, and EMPC$_{NoTerm}$.

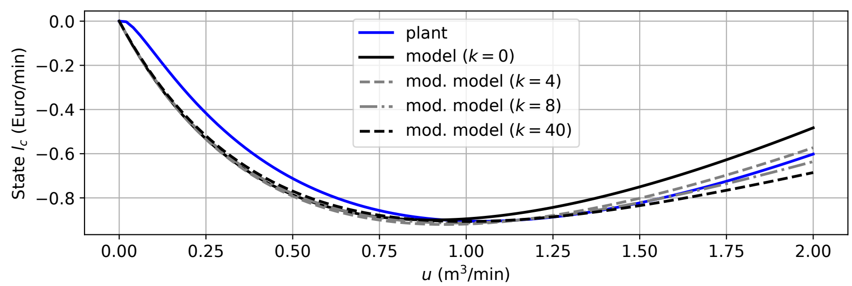

Figure 9: CSTR – Evolution of modified stage cost for EMPC$_{NoTerm}$ at selected time instances $k \in \{0, 4, 8, 40\}$.

Table 3: CSTR – Overview of averaged performance for the control schemes EMPC$_{Nom}$, EMPC$_{MA}$, TMPC$_{MA}$, and EMPC$_{NoTerm}$, $T_{sim} = 15$ min ($N_{sim} = 60$).

N	EMPC$_{Nom}$	EMPC$_{MA}$ ($\sigma = 0.075$)	TMPC$_{MA}$ ($\sigma = 0.2$)	EMPC$_{NoTerm}$ ($\sigma = 0.2$)
16	-0.1815	-0.1828	-0.183	-0.1815
24	-0.1816	-0.1832	-0.1825	-0.1832

Moreover, Table 3 shows the averaged performance of all simulations for $T_{sim} = 25$ min ($N_{sim} = 100$) for two prediction horizons $N \in \{16, 24\}$. As one can see the performance is not affected. Only in case of EMPC$_{NoTerm}$ there appears to be a minor degradation which is likely related to the approximation of the steady-state inputs and adjoints in (24).

Figure 8 shows the trajectories of steady-state input targets $\bar{u}_k$ respectively $\hat{u}_k$ computed via EMPC$_{MA}$, TMPC$_{MA}$, and EMPC$_{NoTerm}$. For EMPC$_{NoTerm}$ we consider three different values of the filter gain $\sigma \in \{0.2,\ 0.4,\ 0.6\}$, while the value for EMPC$_{MA}$ is set to $\sigma = 0.075$ (which is the highest value for which no oscillations of the target steady state occur). This plot confirms that the turnpike-based approximation of the steady-state input and the steady state adjoint (24) is indeed effective.

Finally, Figure 9 shows the evolution of modified steady-state cost $\ell(H_{m,k}(\bar{u}), \bar{u})$ at the time instances $k \in \{0, 4, 8, 40\}$ for the EMPC$_{NoTerm}$ scheme. Here $H_{m,k} : \mathbb{R}^{n_u} \to \mathbb{R}^{n_y}$ is the steady-state input-output map of the modified model at iteration k

$$\bar{x} = f(\bar{x}, \bar{u}), \quad \bar{y} = h(\bar{x}) + \hat{d}_k + \Lambda_k(\bar{u} - \hat{u}_k).$$

As one can see, as the scheme converges to the true plant optimum, the local steady-state approximation of the true plant stage cost improves.

Example 2: non-isothermal Williams-Otto CSTR

As a second, more elaborated, case study we consider the Williams-Otto reactor which is a well-known process control example, also used as benchmark for RTO and MA.[6]

Plant, model, cost and constraints. The Williams-Otto example considered in this study consists of a non-isothermal continuous, stirred-tank reactor in which the following reactions occur in the liquid phase:

$$\begin{aligned}
&\mathrm{A} + \mathrm{B} \xrightarrow{k_1} \mathrm{C}, && r_1 = k_1(T_r)c_A c_B,\\
&\mathrm{B} + \mathrm{C} \xrightarrow{k_2} \mathrm{P} + \mathrm{E}, && r_2 = k_2(T_r)c_B c_C,\\
&\mathrm{C} + \mathrm{P} \xrightarrow{k_3} \mathrm{G}, && r_3 = k_3(T_r)c_C c_P.
\end{aligned}$$

The reactor is fed with a constant flow-rate stream containing species A (rate Q_A, molar concentration c_{A0}) and a variable flow-rate stream containing species B (rate Q_B, molar concentration c_{B0}). The reactor temperature T_r is allowed to vary by adjusting the cooling rate, while the reactor volume V_r is kept constant by setting flow-rate Q_r always equal to the sum of the two inlet flow-rates, i.e. $Q_r = Q_A + Q_B$. Thus, the reactor has two manipulated variables, i.e. Q_B and T_r, while we assume that only the molar concentration of the two desired products, P and E are measured. The kinetic constants follow an Arrhenius type law, i.e. $k_i(T_r) = k_{i0} \exp(-E_i/T_r)$ for $i = 1, 2, 3$ in which T_r is expressed in Kelvin. The process economics is expressed by the following (instantaneous) cost:

$$\ell_c(t) = Q_A c_{A0} p_A + Q_B c_{B0} p_B - Q_r c_P p_P - Q_r c_E p_E, \tag{27}$$

in which p_A, p_B, p_P, p_E are the unit (molar) prices of reactants and products. All process parameters are summarized in Table 4.

Table 4: Williams-Otto Reactor – Process parameters

Parameter	Value	Unit
k_{10}	$9.9594 \cdot 10^6$	$\mathrm{dm}^3/(\mathrm{mol} \cdot \mathrm{min})$
k_{20}	$8.66124 \cdot 10^9$	$\mathrm{dm}^3/(\mathrm{mol} \cdot \mathrm{min})$
k_{30}	$9.9594 \cdot 10^6$	$\mathrm{dm}^3/(\mathrm{mol} \cdot \mathrm{min})$
E_1	6666.7	K
E_2	8333.3	K
E_3	11111	K
V_r	2105	dm^3
Q_{A0}	112.35	$\mathrm{dm}^3/\mathrm{min}$
p_A	7.623	\$/mol
p_B	11.434	\$/mol
p_P	114.338	\$/mol
p_E	5.184	\$/mol

The (mole based) material balances describing the *actual* reactor dynamics are given below:

$$\begin{aligned}
\dot{c}_A &= \frac{Q_A c_{A0} - Q_r c_A}{V_r} - r_1, \\
\dot{c}_B &= \frac{Q_B c_{A0} - Q_r c_B}{V_r} - r_1 - r_2, \\
\dot{c}_C &= -\frac{Q_r c_C}{V_r} + r_1 - r_2 - r_3, \\
\dot{c}_P &= -\frac{Q_r c_P}{V_r} + r_2 - r_3, \\
\dot{c}_E &= -\frac{Q_r c_E}{V_r} + r_2, \\
\dot{c}_G &= -\frac{Q_r c_G}{V_r} + r_3.
\end{aligned} \tag{28}$$

The following constraints should be fulfilled at all times:

$$180\,\mathrm{dm}^3/\mathrm{min} \leq Q_B \leq 360\,\mathrm{dm}^3/\mathrm{min}, \quad 75\,^{\circ}\mathrm{C} \leq T_r \leq 100\,^{\circ}\mathrm{C}. \tag{29}$$

An approximate model is used for EMPC design, which comprises two reactions only

$$\begin{aligned}
&\mathrm{A} + 2\mathrm{B} \xrightarrow{k_1^*} \mathrm{P} + \mathrm{E}, && r_1^* = k_1^*(T_r) c_A c_B^2, \\
&\mathrm{A} + \mathrm{B} + \mathrm{P} \xrightarrow{k_2^*} \mathrm{G}, && r_2^* = k_2^*(T_r) c_A c_B c_P.
\end{aligned}$$

Consequently, the (mole based) material balances describing the *model* reactor dynamics are given below:

$$\begin{aligned}
\dot{c}_A &= \frac{Q_A c_{A0} - Q_r c_A}{V_r} - r_1^* - r_2^*, \\
\dot{c}_B &= \frac{Q_B c_{A0} - Q_r c_B}{V_r} - 2r_1^* - r_2^*, \\
\dot{c}_P &= -\frac{Q_r c_P}{V_r} + r_1^* - r_2^*, \\
\dot{c}_E &= -\frac{Q_r c_E}{V_r} + r_1^*, \\
\dot{c}_G &= -\frac{Q_r c_G}{V_r} + r_2^*,
\end{aligned} \tag{30}$$

in which the kinetic parameters are reported in Table 5.

We note that in this case, the model state has five components $x = \begin{bmatrix} c_A & c_B & c_P & c_E & c_G \end{bmatrix}^\top$

Table 5: Williams-Otto Reactor – Model parameters

Parameter	Value	Unit
k_{10}^*	$1.3134 \cdot 10^8$	$\mathrm{dm}^6/(\mathrm{mol}^2 \cdot \mathrm{min})$
k_{20}^*	$2.586 \cdot 10^{13}$	$\mathrm{dm}^6/(\mathrm{mol}^2 \cdot \mathrm{min})$
E_1^*	8077.6	K
E_2^*	12438.5	K

and differs from the actual plant state $x_p = \begin{bmatrix} c_A & c_B & c_C & c_P & c_E & c_G \end{bmatrix}^\top$. Furthermore, the measured output is $y_p = \begin{bmatrix} c_P & c_E \end{bmatrix}^\top$ and hence the model state vector needs to be estimated from the output.

Comparative study. As in the previous example, we compare the performance of different control strategies:

- Nominal EMPC (EMPC_{Nom}).
- Offset-free TMPC with terminal constraint and $\sigma = 0.2$ (TMPC_{MA}).[8]
- Offset-free EMPC with terminal constraints and $\sigma = 0.2$ (EMPC_{MA}).
- Offset-free EMPC without terminal constraints and $\sigma = 0.2$ (EMPC_{NoTerm}).

In all MPC controllers the model dynamics (30) are integrated with a 4-th order Runge-Kutta method, the chosen sampling time is $h = 0.25\,\mathrm{min}$ and the horizon is $N = 120$, corresponding to $T = 40\,\mathrm{min}$. For all offset-free controllers, we use as disturbance model matrices $B_d = 0$ and $C_d = I$ and as augmented observer gains $K_x = 0$ and $K_d = I$.

Closed-loop inputs and outputs are reported in Figure 10, from which we notice the expected behavior of all controllers: nominal EMPC does not converge to the true plant optimum, while all other controllers converge despite the fact that they use the incorrect model (30).

[8] In this scheme the continuous-time stage cost is $\ell(x,u) = (x - \bar{x}_k)^\top Q(x - \hat{x}_k) + (u - \bar{u}_k)^\top R(u - \hat{u}_k)$, with $Q = I$ and $R = 0.1I$.

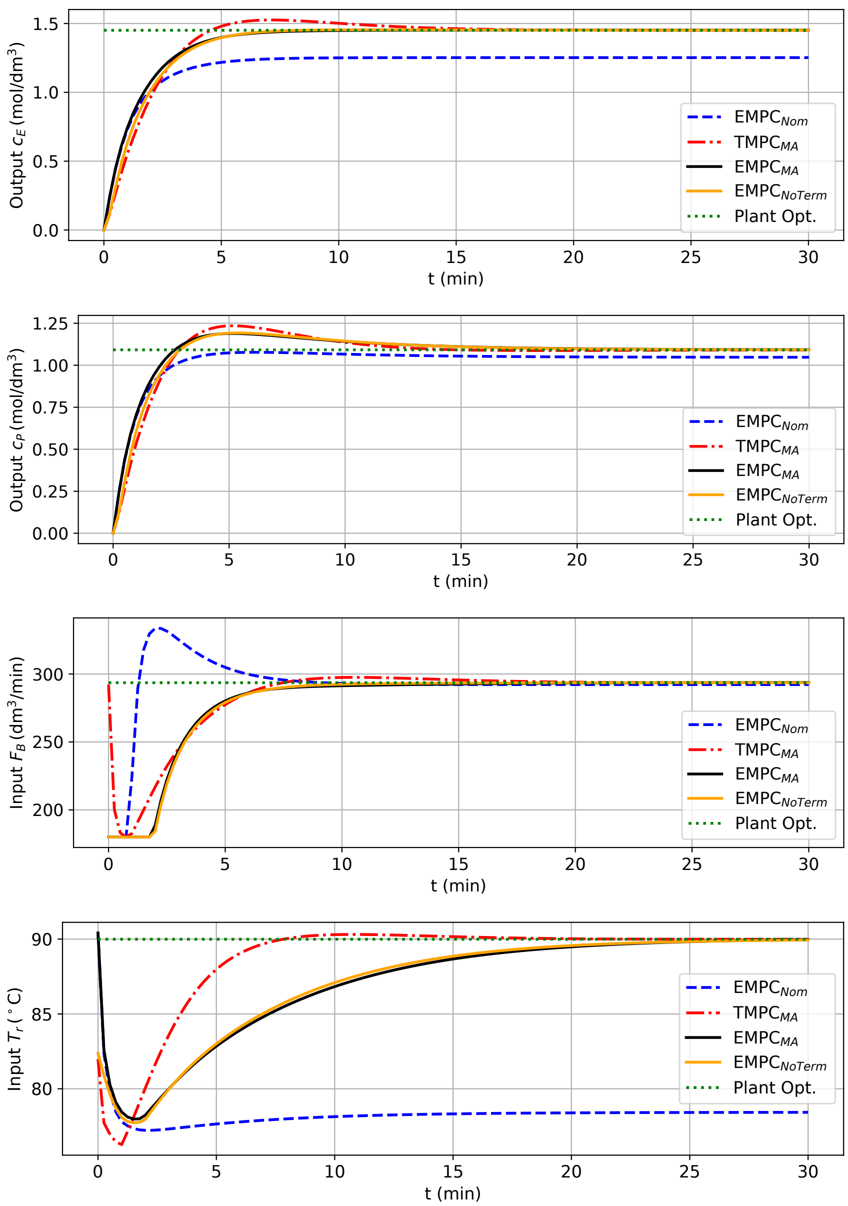

Figure 10: Williams-Otto Reactor – Closed-loop trajectories for the control schemes EMPC$_{Nom}$, EMPC$_{MA}$, TMPC$_{MA}$, and EMPC$_{NoTerm}$.

Figure 11 shows the trajectories of steady-state input targets $\bar{u}_k$ respectively $\hat{u}_k$ computed via EMPC$_{MA}$, TMPC$_{MA}$, and EMPC$_{NoTerm}$, in which for EMPC$_{NoTerm}$ we consider three different values of the filter gain $\sigma \in \{0.2, 0.4, 0.6\}$. Also in this case, we note that the turnpike-based approximation of the steady-state input and the steady state adjoint (24) is very effective.

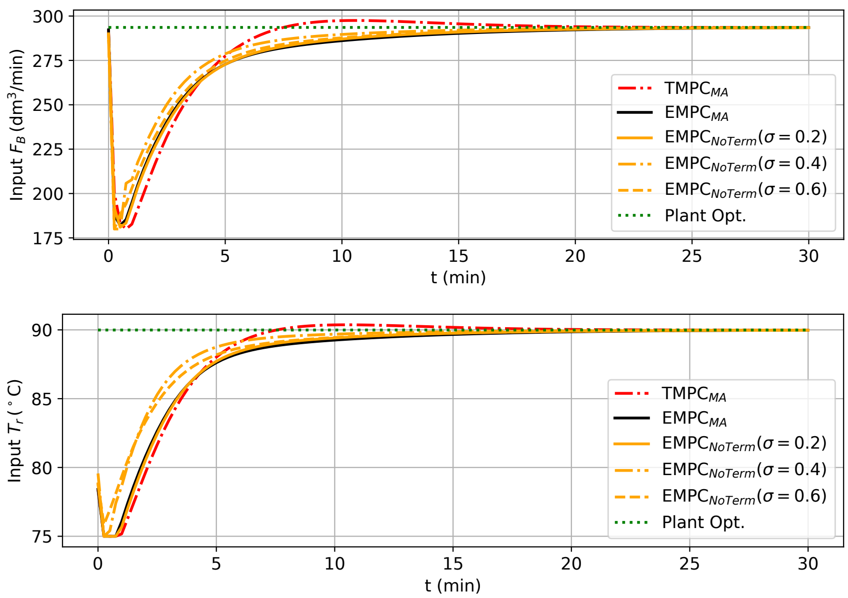

Figure 11: Williams-Otto Reactor – Trajectories of steady-state input targets $\bar{u}_k$, respectively, $\hat{u}_k$ for the control schemes EMPC$_{MA}$, TMPC$_{MA}$, and EMPC$_{NoTerm}$.

Finally, the averaged performance of all control strategies, using different prediction horizons, is compared in Table 6. As in the previous example, we notice that the turnpike-based approximation of steady-state input and adjoint does not induce a relevant degradation of performance.

Table 6: Williams-Otto Reactor – Overview of averaged performance for the control schemes EMPC_{Nom}, EMPC_{MA}, TMPC_{MA}, and EMPC_{NoTerm}, $T_{sim} = 30$ min ($N_{sim} = 120$).

T/N	EMPC_{Nom}	EMPC_{MA} ($\sigma = 0.2$)	TMPC_{MA} ($\sigma = 0.2$)	EMPC_{NoTerm} ($\sigma = 0.2$)	EMPC_{NoTerm} ($\sigma = 0.4$)	EMPC_{NoTerm} ($\sigma = 0.6$)
20/80	-142.1	-193.5	-184.4	-189.1	-190.4	-191.0
25/100	-140.8	-192.8	-184.4	-188.74	-190.0	-190.6
30/120	-140.8	-192.54	-184.4	-188.54	-189.8	-190.36

Outlook and Conclusions

This paper has investigated the combination of RTO and economic MPC. We have provided a conceptual framework to blend concepts from modifier adaptation into economic MPC. Specifically, we propose combining three main elements: an augmented state estimator, which provides estimates of the slowly varying offsets on states and outputs, estimation of plant gradients and a tailored formulation of the OCP to be solved at each MPC iteration. In the OCP we suggest using a recently proposed formulation considering a gradient correcting end penalty and no terminal constraints. Our results show that, provided the open-loop optimal solutions of the OCP exhibit the turnpike phenomenon, then it is possible to avoid any explicit computation of steady-state targets from the picture. Instead, the required quantities—i.e. estimates of the optimal steady state input and of the steady-state adjoint—can be obtained from the open-loop optimal predictions.

Interestingly, in comparison to the combination of tracking MPC with modifier adaptation and to offset-free EMPC with terminal constraints, the proposed scheme delivers equivalent performance while being conceptually much simpler. Unsurprisingly (at least from the RTO perspective) our results illustrate that the crucial element in combining RTO and MPC is the estimation of steady-state plant gradients.

While the present paper has focused on conceptual ideas, future work will investigate the formal analysis of the proposed scheme.

Acknowledgement

The present paper is dedicated to Dominique Bonvin. His contributions have pushed the frontiers in real-time optimization of uncertain process systems over several decades. Specifically, the paper combines (output) Modifier Adaptation[5,6,44] with the insights into the structure of solutions to optimal control problems[73]—such as turnpike properties[43,53]—and economic MPC.[56,66] Put differently, this paper leverages ideas and concepts advocated by Dominique Bonvin throughout his career.

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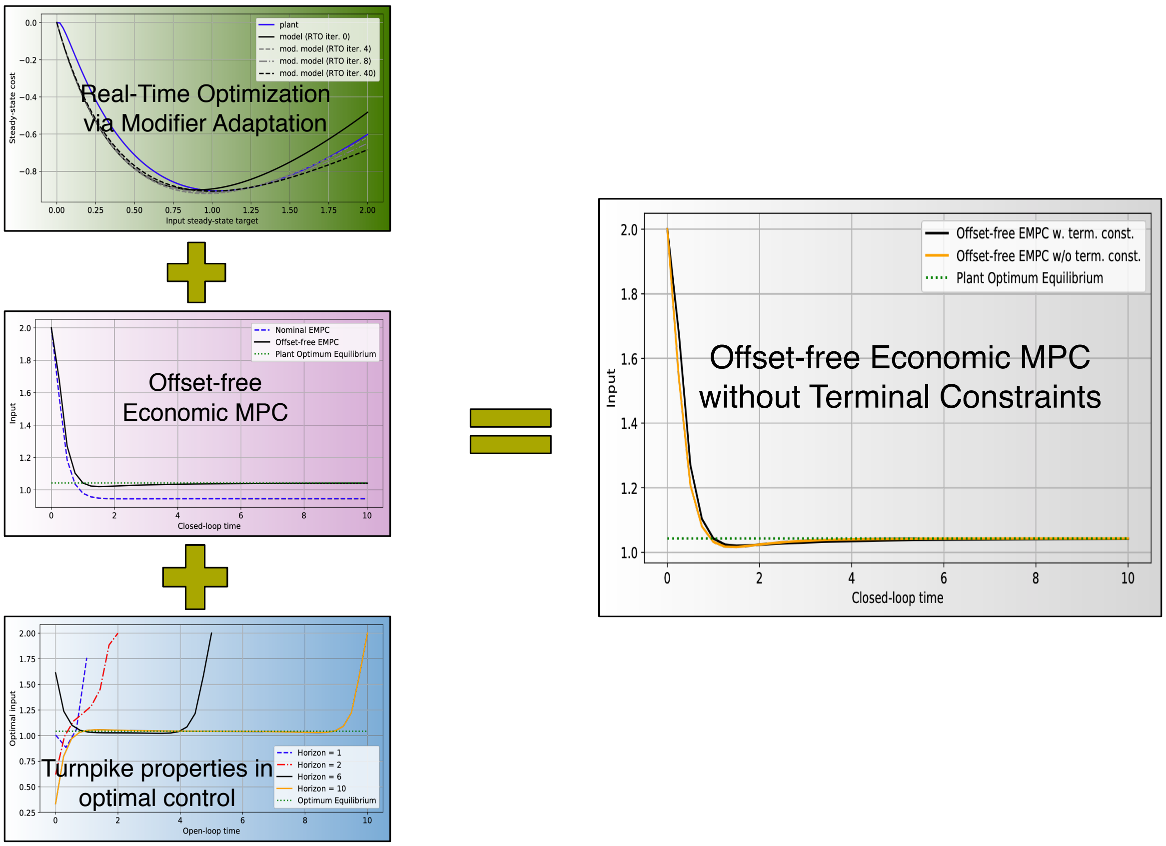
TOC graphic



Real-Time Optimization via Modifier Adaptation
plant
model (RTO iter. 0)
mod. model (RTO iter. 4)
mod. model (RTO iter. 8)
mod. model (RTO iter. 40)
Steady-state cost
Input steady-state target
Offset-free Economic MPC
Nominal EMPC
Offset-free EMPC
Plant Optimum Equilibrium
Input
Closed-loop time
Turnpike properties in optimal control
Horizon = 1
Horizon = 2
Horizon = 6
Horizon = 10
Optimum Equilibrium
Optimal input
Open-loop time
Offset-free Economic MPC without Terminal Constraints
Offset-free EMPC w. term. const.
Offset-free EMPC w/o term. const.
Plant Optimum Equilibrium
Input
Closed-loop time