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Abstract:

This document provides a report on market-based coordination strategies developed in the Workpackage (WP) 2 of the DYMASOS project. We present a subset of problems arising typically in processing industries, related to the case studies defined in the WP 5 of the project. We briefly review the approaches, present in the literature, based on market-like coordination mechanisms that steer the behavior of the constituent systems of a (cooperative) system of systems to fulfill a common goal under present coupling in the form of shared resources. We present the developments which provide extensions to the state-of-the-art methodologies of price-based coordination. These, on one hand, establish efficient (fast-convergent) price-based coordination and, on the other hand, enlarge the domain of applicability of this type of coordination to problems involving non-strictly convex objective functions of local management problems, stringent local constraints, and discontinuous production units. This report also discusses the implementation of the proposed algorithms into the simulation platform that is developed in WP 4 of the DYMASOS project. This implementation allows for seamless transition of the research presented here to action at the real-world engineering problems. Several examples, of varying complexity, are provided to illustrate the basic features of the reported methods and give a concrete outlook of the applications of these methods for the case studies of DYMASOS.

Keywords:

Dynamic management, Systems of systems, Market-based coordination, Production optimization.

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The DYMASOS Project

The well-being of the citizens in Europe depends on the reliable and efficient functioning of large interconnected systems, such as electric power systems, air traffic control, railway systems, large industrial production plants, etc. Such large systems consist of many interacting components. The sub-systems are usually managed locally and independently, according to different policies and priorities. The dynamic interaction of the locally managed components gives rise to complex behaviour and can lead to large-scale disruptions as e.g. black-outs in the electric grid.

Large interconnected systems with autonomously acting sub-units are called systems of systems. DYMASOS addresses systems of systems where the elements of the overall system are coupled by flows of physical quantities, e.g. electric power, steam or hot water, etc.

Within the project, new methods for the distributed management of large physically connected systems with local management and global coordination will be developed.

The **DYMASOS Consortium** consists of:

Participant No.	Participant Organisation Name	Participant Short Name	Country
1	Technische Universität Dortmund	TUDO	Germany
2	BASF SE	BASF	Germany
3	HEP-Operator distribucijskog sustava d.o.o	HEP	Croatia
4	INEOS Köln GmbH	INEOS	Germany
5	University of Seville	USE	Spain
6	University of Zagreb Faculty of Electrical Engineering and Computing	UNIZG-FER	Croatia
7	ETH Zürich	ETH	Switzerland
8	RWTH Aachen University	RWTH	Germany
9	inno TSD	inno	France
10	Optimizacion Orientada a la Sostenibilidad SL	IDENER	Spain
11	euTeXoo GmbH	TEX	Germany
12	Ayesa Advanced Technologies SA	Ayesa AT	Spain

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1. Introduction

According to Maier [1], the characteristic features of systems of systems (SoS), as opposed to traditional concept of systems, are:

- Operational and managerial independence
- Geographic distribution
- Evolutionary behavior
- Emergent behavior

The DYMASOS project mainly focuses its studies and applications on tackling the first listed point. Modern large-scale, complex technical systems, such as smart grids, railway systems, or integrated industrial production sites, consist of many, partly autonomous, physical and cyber components with complex interactions. These features classify these systems as SoS. In most cases there exist physical couplings among the constituent systems of SoS, such as flows of material or energy. These couplings must be considered when one seeks the optimal operation and management of the SoS. As the components of SoS possess partial autonomy, their actions must be, in many cases, coordinated in order to steer the SoS towards operational excellence and effectiveness, i.e. optimality. Architectures for the optimal coordination of the SoS must be able to deal with the large size and complexity of these systems for which centralized solutions of the optimal operation and management problems may be infeasible. Thus, distributed solutions are often favored by engineers and managers.

1.1 Operational Independence of Systems of Systems and Process Industry

This deliverable deals with distributed optimization problems that arise in the management of physically-coupled systems of systems in continuous production units where we focus our attention on the process industries.

In the process industries, energy and resource efficiency is a central concern, both for economic reasons and in order to reduce the carbon footprint and to ensure long-term sustainable production. Energy and resource efficiency are mainly determined by the design of the plants, but the way in which they are operated has a significant influence as well. Model-based real-time optimization (RTO) [2] or model-based optimizing control [3] are increasingly applied to improve the operations in the presence of disturbances, changing feeds and changing demands. The scope of these technologies is, however, restricted to single plants within a larger site. In many cases, as in large chemical sites, the plants are connected by networks of resources, e.g., steam on different pressure levels, hydrogen, or intermediates. Due to this coupling the local optima may not be the best operating points for the overall site. So a site-wide optimization is of interest, but this often cannot be realized mainly due to three reasons:

- the overall problem becomes too large to be solved efficiently
- centralized solutions are vulnerable to missing or unreliable information
- the plants may belong to different business units or even to different companies which do not want to share the models and economic performance indicators.

Therefore distributed and hierarchical optimization methods are of interest [4].

The distributed optimization problem represents the site-wide optimization problem where the local subsystems (production or business units, plants) solve their own local management problems, i.e. they perform local optimization to find the best operating point or utilization of time-varying degrees of freedom (dynamic inputs) for the current situation at the plant and current signals from upper management levels (product demands, product and feedstock

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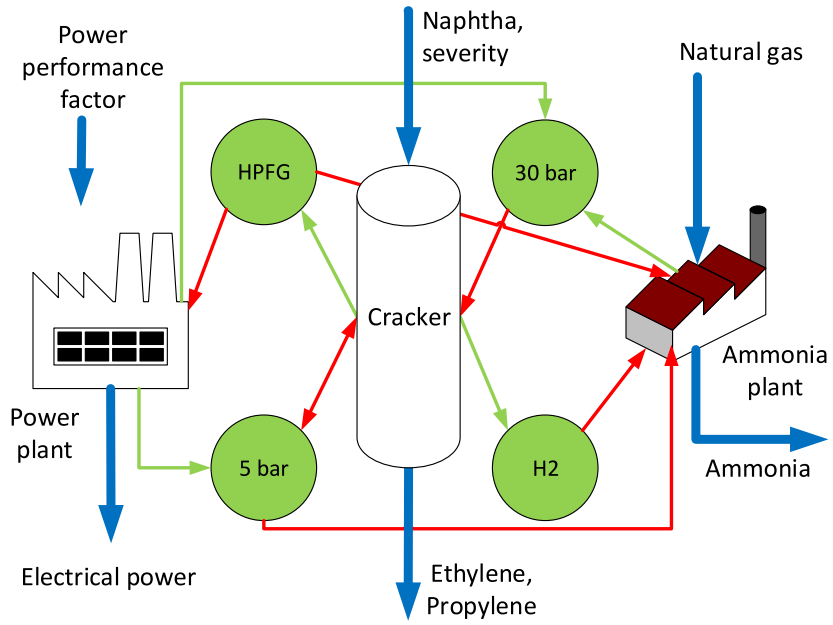

Figure 1: A part of the production site extracted from INEOS case study.

prices, etc.). The subsystems have their individual objective functions and also local constraints, but they share some common constraints which represent the shared resources and intermediates being consumed and produced at the site.

For instance, consider a problem of site-wide optimization as studied in the DYMASOS case study provided by partner INEOS. A part of the site involving cracker, ammonia and power plant is depicted in Fig. 1. This problem is studied in [5]. A global (overall) objective function is given that optimizes the profit of the site that is composed of the profits of individual units such that

$$J(u_1, u_2, u_3) = J_1(u_1) + J_2(u_2) + J_3(u_3), \tag{1.1}$$

where three separable objectives represent the production profit of the three plants and the decision variables u_i stand for the operational degrees of freedom of the plants. It is quite common that, in practice, the optimization of plants' (local) objectives is done in distributed fashion, i.e. the local objectives are optimized by separate entities (business unit managers, agents) separately since the local degrees of freedom can only be adjusted locally. There exists then a central coordination authority which ensures that the networks of shared resources (raw materials, energy, intermediates) are balanced and that the demand of the shared resources does not surpass the supply. For the INEOS case study, this represents achievement of the balance of steam networks (5 bar and 30 bar), fuel gas (HPFG) and hydrogen (H_2) depicted in Fig. 1.

The described problem can be considered as three subproblems with local objectives $J_1(u_1)$, $J_2(u_2)$ and $J_3(u_3)$, each of which may have its local constraint functions. A characteristic feature of processing plant complexes is that the units are coupled by networks of utilities, e.g. steam, electricity, cooling water or raw materials. In these complex networks, the units can act as consumers and producers of resources. The utilization of these shared resources has to be coordinated between the distributed structures in order to fulfill the global demand-supply constraints for each shared resource network. Consequently the global problem is also subject to some global constraint functions (e.g. $G_1u_1 + G_2u_2 + G_3u_3 = g$) that couple the variables of the local problems. The parameters (or functions) G_1, G_2, G_3 represent the producing or consuming character of the plant w.r.t. to shared resources and g stands for external demand or supply in case of import or export of the resources out of the balance volume of the site.

Besides the operational independence originating from the local character of the decisions (decisions only affect the local unit), another reason for distributing the centralized problem are privacy issues. Different processing plants may be operated by different business units of a company or even by different companies in a chemical park which do not make all the details of their operational constraints, costs, and profits transparent. In such a situation, local decision makers are responsible for the operation of the individual plants, and global coordination has to be achieved by a mechanism that possesses only limited information about the subsystems.

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This report mainly focuses on the distributed optimization in the framework of RTO and MPC (Chapters 2 and 3).

In the process industries, many products are produced in several parallel-running semi-batch reactors due to the high flexibility in terms of amount, product type, and product specifications. These reactors usually share networks of resources, e.g. the feed flow rate, cooling water, etc. Similarly to the problem of production coordination of continuously operating units, the dynamic optimization (determination of the best batch recipe) should take into account the balance of the shared resources and the repetitive character of production, i.e. once the batch is finished, the reactor will be utilized for running another batch. In case of many batches that run in parallel the optimal consecutive-batch operation can be found by employing a cyclic constraint formulation. This formulation can then be casted as a local optimization of the individual reactors with hierarchical coordination scheme that ensures the fulfillment of shared-resource constraints. We devote the Chapter 4 of this report to study this problem.

1.2 Algorithms for Coordination of Coupled Continuous Production Processes

Decomposition strategies are key components of many methods that look for the solution of large-scale optimization problems where subsystems that share some resources can be identified. The decomposition is applied to divide the original problem in subproblems whose solutions depend on some coordination variables (such as prices or multipliers) that are available as an information to each subsystem and computed in the upper coordination layer in order to satisfy the global constraints and to achieve desired optimal performance of the system.

Different techniques can be found in the literature for distributed and hierarchical optimization [6] depending on the degree of autonomy of the constituent systems, e.g. whether systems assign some of their degrees of freedom using a local management (optimization), and based on the overall system architecture, e.g. whether there exists a central entity that can coordinate the local decisions by issuing some global reference signals. Among these techniques price-based optimization has been identified as a promising candidate for a realization of distributed management in process systems [7].

One of the first decomposition strategies ever developed is the Dantzig-Wolfe (DW) decomposition [6]. This method can be classified as a distributed simplex algorithm and can be used for efficient solution of the linear programming problems where the constraints structure is sparse such that there exists a subset of constraints of joint (where almost every variable occurs) and local (where only few variables occur) character. This technique is very appealing for the practical implementation as it was shown to be very efficient [8]. Some applications also include coordination of distributed industrial model predictive control (MPC) controllers [9]. The advantage of DW decomposition is that the coupling constraints are relaxed and enforced by coordinator that iteratively finds and broadcasts the values of Lagrange multipliers of the coupling constraints, which can be interpreted as transfer prices. This feature makes it suitable for the desired coordination mechanism, as discussed above. The downside of the DW algorithm is that the coordinator requires information about the local constraints of the subsystems so the aforementioned privacy restrictions are violated if this method is in use.

The price-based coordination can be realized through application of the dual decomposition approaches [7, 10, 11, 12, 13]. These techniques are also suitable for the application in model predictive control (MPC) of interconnected units [14, 15, 16]. The general procedure in these approaches can be interpreted through market theory and resembles a Walrasian auction in which the central site management takes the role of an auctioneer and the local optimizers are the agents that take part in the auction [17]. The auctioneer iteratively sets prices until the demand and the supply of the agents match. To apply this interactive process, the local objectives are assumed to depend on the prices of shared resources. The Lagrange multipliers can thus be interpreted as transfer prices that either incur costs for the local plants, when these consume resources, or they create a reward for the production of resources [4].

In price-based coordination approaches, prices for the utilization of the coupling constraints enter into the local optimization problems and a central coordinator influences the local optimization by manipulating the price in the same way as in an open market. These algorithms usually only require information about the local utilization of the shared resources, which makes them attractive to the industry where the different economic operators that do not

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want to make the detailed knowledge of their internal operation public. The current practice for balancing of production and consumption of shared resources in petrochemical sites is through direct negotiation of the prices of the shared resources between the management of the different business units, resulting in an internal micro-market. This points to a potential of market-based algorithm, but, although the theory of market exchange is old [17], the number of successful examples of the application of such methods to problems from the process industry is limited [10, 11, 12, 18, 19, 20].

In [10, 21], the authors propose a solution based on multi-agent systems for a distributed resource allocation in technical or industrial environments. They refer to a mathematical formulation of the resource allocation problem as an optimization problem and use this formulation to derive the local behavior and the interaction behavior of the agents. The novelty presented here is the combination of market-based mechanisms for resource allocation and process control in continuous production.

In [11], the authors propose a price-based coordination framework for distributed MPC applications that can be formulated as a large-scale quadratic program with linking equality constraints. The price adjustment algorithm is based on the Newton's method and employs sensitivity analysis and active set change identification techniques. The proposed decentralized MPC framework is tested across several case study examples and the results are promising in providing an acceptable on-line calculation speed for solving industrial plant-wide MPC optimization problems.

In [22] the authors present a coordinated-distributed control scheme for discrete-time linear process systems. This scheme employs local model predictive controllers that can be coordinated to achieve the centralized optimal performance. For coordination of the local controllers, the authors propose price-based mechanisms and they combine price-driven decomposition [23] with Newton's method along with a sensitivity analysis technique to update the Lagrange multipliers. Through simulations performed on a fluid catalytic cracking benchmark process coupled by inputs and the states, the authors show that the proposed method provides rapid convergence towards the plant-wide optimum.

Similar work has been done in [20] where the authors present successful implementation of the decentralized NMPC coordination architecture on a laboratory scale oxygen distribution network. The price-based coordination algorithms need less time to calculate the plant-wide optimal inputs compared to the centralized scheme and converge to the plant-wide optimum unlike the completely decentralized architecture. They extend their work and compare different tuning techniques for the price coordination as presented in [12] where it is shown that using market-based algorithms are superior in price adjustment compared to PI algorithm or heuristic algorithms.

In [24], the authors present the mathematical conditions under which a system-level optimization of supply and demand scheduling can be implemented as a distributed optimization in which users and suppliers, as well as the load serving entities, are decision makers with well-defined partial objectives using price-based coordination. The requirements for convergence of the global objectives and the local/individual objectives are defined and novel algorithms for coordinating of the supply-demand problems on different time scales like day ahead horizon and real time adjustment are developed.

Some further studies that touch on the topic of price-based coordination can be found in:

- [22, 25, 26, 27, 28] for problems involving linear models
- [12, 29, 30] for non-linear problems
- [31, 32] for limited communication bandwidth
- [33, 34, 35, 36] for general cooperative problems and consensus problems

While the price-based coordination reduces the size of the problem of site-wide optimization and ensures the confidentiality of the information among the constituent plants, one of the main obstacles towards the industrial application of the technique is the slow rate convergence rate [37]. In order to address these issues, we present, in this report (Chapter 3), a new scheme for the price-based coordination.

In the recent years, different approaches for solving plant-wide optimization problems have been proposed and one of the most promising algorithms is the Alternating Direction Method of Multipliers (ADMM). ADMM is popular for

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different type of decomposition problems and an extensive summary of the characteristics and the applications is presented in [4]. The main advantage of ADMM lies in the fact that the convergence of the algorithm can be proven under mild assumptions. The ADMM does not require strict convexity of the objective functions of local optimization problems as opposed to dual decomposition applied, normally, for price-based coordination. The ADMM is also guaranteed to converge for nonlinear convex models [38]. The difference of ADMM w.r.t. dual decomposition is the modification of local optimization problems such that an augmented-Lagrangian formulation is employed.

Although the method originates from the 1950s, and was fully developed in the 1970s, the authors in [39] argue that ADMM is still well suited for distributed convex optimization, and in particulate to large-scale problems. The performance of ADMM versus different state-of-the-art decomposable convex quadratic programming methods employing duality has been investigated in [39]. In [26], the authors propose ADMM-based decomposition of the model predictive control algorithm. The MPC problem is transferred to a separable formulation with the use of an indicator function and by introducing extra consensus constraints. This formulation employs the projected gradient descent ADMM and therefore leads to relative short computation times.

One of the greatest challenges of the ADMM algorithms is the slow convergence, and a many researches are devoted to designing modifications that improve the ADMM convergence rate in specific situations [40]. The selection of the step size of the dual variables update is crucial for the convergence rate of ADMM. One possible way to define the optimal step size is presented in [41, 42], where the focus is on the application of ADMM to the QPs of constrained MPC. The authors provide a proof of convergence using the theory of maximal monotone operators. The result allows relaxation of the existing assumptions in optimal step size selection, that limit the applicability to the QPs of MPC. Very similar research is conducted by the authors in [43, 44]. They derive explicit analytic expressions for the optimal convergence factor and the optimal step-size for different formulations of the ADMM algorithm.

Although ADMM is largely used to solve large-scale linearly constrained optimization problems, the majority of theoretical results relate to quadratic and convex functions. Recently some authors analyze the convergence properties of ADMM for solving certain class of non-convex consensus and sharing problems. In [29] the authors show that the classical ADMM converges to the set of stationary solutions, if the penalty parameter in the augmented Lagrangian is chosen to be sufficiently large.

We study the application of ADMM in price-based coordination for resource-sharing and consensus problems. The presented cases studies include distributed MPC problem for shared resource allocation (INEOS case study of the DYMASOS project in Chapter 3) which involves linear (non-strictly convex) local objective functions and sharing and consensus problem of coupled batch reactors which involve nonlinear dynamics (Chapter 4).

1.3 Engineering Support for the Implementation of Coordination Strategies

The development and deployment of novel coordination methods for distributed management and control, as they are described in this study, into practical application poses several engineering challenges for which tool support is under development in WP4 of the DYMASOS project. The development of coordination methods requires a means to validate their performance and correctness, which is usually done by testing based on a simulation model of the system under consideration. This model may consist of many model components, some of which may already exist, e.g. they might be implemented in different tools. Thus, a tool for simulation-based validation must be able to seamlessly accommodate proprietary and black-box models, e.g. using co-simulation, and provide standardized interfaces to which the management algorithms and the different types of models can be connected. This plug-and-play capability will allow the engineers to easily connect or change simulation models, facilitating model re-use, and will facilitate the deployment of distributed coordination methods to industrial hardware.

In this report we present how the generic framework developed in DYMASOS project can be used to simulate and validate the coordination of distributed architectures. The framework is based on the Modelica language for heterogeneous modeling (see e.g. [45]) and aims at reducing the effort for model creation by providing standard interfaces for the connection of physical process model components with different levels of detail (both existing and newly

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developed models) as well as management algorithms. Its applicability is demonstrated by connecting a distributed MPC control structure to the simulation model of a four-tank benchmark problem (Chapter 2) and INEOS case study (Chapter 3).

1.4 Structure of this Report

The rest of this deliverable is organized as follows. First, in Chapter 2, priced-based coordination is explained and linked to the general formulation of an optimal resource allocation problem and an optimal consensus problem. An optimal consensus problem is studied in the framework of distributed MPC and the results are illustrated on a benchmark problem taken from the literature. The main purpose of the chapter is to evaluate the performance of price-based coordination in the presence of local constraints of the constitutive subsystems of system of systems and to showcase the implementation of price-based coordination in the modeling, simulation and validation framework developed in the DYMASOS project. Chapter 3 presents the extensions developed in WP2 of the DYMASOS project that enhance the convergence of the price-based coordination using the quadratic-approximation techniques and that extend the applicability of the price-based coordination beyond the strictly convex nature of the underlying local optimization problems using the ADMM. These developments are illustrated on a prototypical problem of sharing the resources in an integrated production complex and on a steam management problem extracted from the INEOS case study. Finally it is shown in Chapter 4 how the market-based mechanisms can be applied for the coordination of discontinuous (batch) production systems. The solution of the problem, which is structurally similar to the BASF case study, is demonstrated on a benchmark problem.

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2. Market-based Coordination for Continuous Production Units

This chapter introduces the problem of distributed management, explains the principle of coordination using price-based mechanisms and illustrates the application and implementation of price-based coordination on a benchmark problem of distributed model predictive control (MPC).

2.1 Problem Description and Coordination Principle

We study the problem of optimal management of system of systems that can be expressed in the following form

$$\min_U \sum_{i=1}^{n} J_i(u_i) = \min_U \sum_{i=1}^{n} \frac{1}{2} u_i^T H_i u_i + w_i^T u_i \tag{2.1a}$$

$$\text{s.t.} \sum_{i=1}^{n} G_i u_i = g, \tag{2.1b}$$

$$L_i u_i \leq l_i, \qquad \forall i \in \{1, \ldots, n\}, \tag{2.1c}$$

with $J_i : \mathbb{R}^{m_i} \to \mathbb{R}$ denoting the cost function of plant i, symmetric positive definite matrices $H_i \in \mathbb{R}^{m_i \times m_i}$ and matrices $G_i \in \mathbb{R}^{g \times m_i}$ and $L_i \in \mathbb{R}^{l_i \times m_i}$. The decision variables of the problem $U := (u_1^T, \ldots, u_n^T)^T$ represent the degrees of freedom of the local problems, i.e. operational decisions or inputs in the presence of local dynamics. Note the separable nature of the objective function (2.1a). This structure suggests that the decision of the ith agent can be reached independently (e.g. in parallel fashion) of the rest of the agents. This separation (decentralization) establishes a notation of a local optimizer of the unit (plant) i which pursues its own production or managerial goal. The conditions (2.1c) represent the local constraints of each individual agent (plant). The constraints (2.1b) represent couplings among the subsystems which have to be respected by the individual optimizers. Hence these constraints pose the only obstacle for complete decentralization of the problem.

In this report we consider the cases where the coupling constraints can take two principal forms.

- Resource-limiting constraints (Resource allocation problem)

  Often, a central site management of an industrial production complex has to allocate shared resources among different competing agents—these can be either single productions units or business units—which have managerial autonomy in terms of their local operation (see Fig. 2). A centralized optimization of the production site thus involves evaluation of the local economic costs as well as a global constraint reflecting the network balance. The centralized optimization problem reflecting the structure is depicted in Fig. 2. The constraints of this problem can be formulated as

  $$\sum_{i=1}^{n} R_i + R_e = 0, \tag{2.2}$$

  which comprises the sum of the n shared resource utilization vectors $R_i \in \mathbb{R}^g$ and the external flows R_e that are leaving or entering the balance space. Such external flows can be intermediate product streams that are sold to other parts of the production site, which are not considered in the balance space, as well as imported or exported utilities like electric power to the grid. These constraints can clearly be reformulated into the form of (2.1b) if, as usual scenarios suggest, the dependence of the shared resources is linear in the decision variables of the ith plant, i.e. $R_i = G_i u_i + r_i$. Here a supply of a plant to the shared resource network is denoted with a negative sign ($R_{i,j} < 0$), while a consumption is represented by a positive quantity ($R_{i,j} > 0$), with j as the index of a particular shared resource. The right-hand side of (2.1b) becomes

  $$g = -R_e - \sum_{i=1}^{n} r_i,$$

  under this reformulation.

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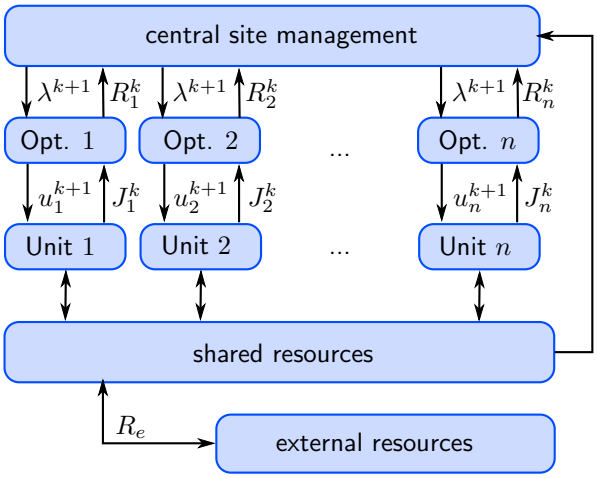

Figure 2: A typical management structure of a large industrial complex with distributed optimizers (Opt. i) and (partially) autonomous plants (Units i), coupled by shared resources.

- Consensus constraints (Global consensus problem)

  A mutual agreement among the constituent systems of system of systems can be sought upon certain quantities. The examples include trajectory following of the autonomous ground, marine and aerial vehicles or frequency adaptation in power grids. We show an application to the coordination of the production of discontinuous (batch) production units in Chapter 4 of this report. The so-called consensus constraints take the form

$$u_1 = u_2 = \cdots = u_n. \tag{2.3}$$

  Note that it can be assumed that $m_1 = m_2 = \cdots = m_n = m$ in this case. In the form of (2.1b), they can be stated using

$$g = 0, \qquad G_1 = \begin{pmatrix} \mathbf{I}_m \\ \mathbf{0}_{m\times(n-2)} \\ -\mathbf{I} \end{pmatrix}, \qquad G_i = \begin{pmatrix} \mathbf{0}_{m\times(i-1)} \\ -\mathbf{I} \\ \mathbf{I} \\ \mathbf{0}_{m\times(n-i)} \end{pmatrix}, \ \forall i \in \{2,\dots,n\}, \tag{2.4}$$

  where $\mathbf{I}_m$ represents the m-dimensional identity matrix and $\mathbf{0}_{r\times c}$ is a zero matrix with r rows and c columns.

2.1.1 Problem Decomposition and Hierarchical Coordination by Price-based Mechanisms

The optimality conditions of the problem (2.1) may be formulated using the Lagrange function

$$\mathcal{L}(u_1,u_2,\dots,u_n,\lambda,\nu_1,\nu_2,\dots,\nu_n) = \sum_{i=1}^{n}\left(\frac{1}{2}u_i^T H_i u_i + w_i^T u_i + \lambda^T G_i u_i + \nu_i^T(L_i u_i - l_i)\right) - \lambda^T g, \tag{2.5}$$

where ν and λ represent the vectors of Lagrange multipliers associated with local and global constraints respectively.

Using (2.5) the optimality conditions of problem (2.1) then read as

$$0 = \nabla_{u_i}\mathcal{L} = H_i u_i + w_i + G_i^T\lambda + L_i^T\nu_i, \tag{2.6a}$$

$$0 = \nabla_{\lambda}\mathcal{L} = \sum_{i=1}^{n} G_i u_i - g, \tag{2.6b}$$

$$0 = \nu_{ij}L_{ij}u_i, \quad L_i u_i \le l_i, \quad \nu_{ij} \ge 0, \quad \forall i \in \{1,\dots,n\},\ \forall j \in \{1,\dots,l_i\}. \tag{2.6c}$$

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It is a common approach to assume that the local constraints are not active at the optimum and that only the coupling constraints determine the optimum [10, 20, 46]. This is equivalent to taking $\nu_{ij} = 0$, $\forall i \in \{1, \ldots, n\}$, $\forall j \in \{1, \ldots, l_i\}$. We will make a similar assumption, however, unlike other studies, we will assess the effect of the presence of the local constraints in this report.

If the constraints (2.6b) are relaxed, the optimization problem (2.1) can be decomposed into n local optimization problems of the form

$$\min_{u_i} \frac{1}{2} u_i^T H_i u_i + w_i^T u_i + \lambda^T G_i u_i \tag{2.7a}$$

$$\text{s.t. } L_i u_i \leq 0. \tag{2.7b}$$

Hence the presence of a penalty term $\lambda^T G_i u_i$. This is introduced in order to fulfill the optimality conditions (2.6a). The vector of Lagrange multipliers λ is common to all n optimization problems and, because of the structure of (2.7a), it can be interpreted as prices of the shared resources or incentives to reach the global consensus. Hence the name price-based coordination.

While on the (lower) level of the local optimizers the optimization problems are solved in decentralized fashion, the central coordinator is needed to iteratively adjust the prices in order to drive the local systems to the satisfaction of coupling constraints (e.g. to reach balanced networks of the shared resources). This can be reached using the dual function of the optimization problem (2.1), which can be expressed as

$$d(\lambda) = \min_u \mathcal{L}(u, \lambda). \tag{2.8}$$

To find the update of the price vector λ^{k+1} the old price vector is corrected with the gradient of the dual function.

$$\lambda^{k+1} = \lambda^k + \alpha^k \nabla d(\lambda^k), \tag{2.9}$$

where $\alpha^k \in \mathbb{R}$ is the step size parameter. In practice is is not always straightforward to find this direction (e.g., when the functions are not differentiable [47]). In this case the update step can be defined using the subgradient ∂d.

$$\lambda^{k+1} = \lambda^k + \alpha^k \partial d(\lambda^k). \tag{2.10}$$

For the problem at hand the subgradient is the residual of the constraints functions (2.1b), which can be written as

$$\partial d(\lambda^k) = \sum_{i=1}^{n} G_i u_i^{*,k} - g, \tag{2.11}$$

where u_i^* denotes the optimal operating point of subsystem i for the price vector λ^k. From (2.11) it can be seen that the prices are updated as long as the constraints are not satisfied. As soon as they are fulfilled the equilibrium price λ^* is attained—similar to the market-clearing price in market theory.

Using Newton's method to fulfill the conditions (2.1b), the coordinator problem becomes

$$\lambda^{k+1} = \lambda^k + \left(\sum_{i=1}^{n} G_i H_i^{-1} G_i^T \right)^{-1} \left(\sum_{i=1}^{n} G_i u_i - g \right), \tag{2.12}$$

which shows a proper selection of α^k if the coordinator possesses the required information about the subsystems. We will assume in this chapter this information is available to the coordinator. The next chapter then discusses an approach how the coordinator can iteratively attain this knowledge.

In summary, the principle of the price-based coordination is then following. The coordinator transfers the price vector λ to the subsystems and collects the responses g_i, $\forall i \in \{1, \ldots, n\}$. Based on this information it decides about the new update and this process repeats itself until the primal feasibility condition (2.1b) is fulfilled, i.e. the optimality conditions (2.6a) are satisfied.

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2.2 Demonstration Example

We consider the problem of distributed MPC for n systems where the centralized control problem reads as

$$\min_{X,U} \sum_{i=1}^{n} \sum_{j=k}^{k+N_p-1} \|x_i(j+1) - x_i^{\mathsf{r}}(j+1)\|^2_{Q_{x,i}} + \|u_i(j) - u_i^{\mathsf{r}}(j)\|^2_{Q_{u,i}} \tag{2.13a}$$

$$\text{s.t. } (\forall i = 1,\dots,n,\ \forall j = k,\dots,k+N_p-1):$$

$$x_i(j+1) = A_i x_i(j) + B_i u_i(j), \tag{2.13b}$$

$$\sum_{i=0}^{n} \tilde{G}_i (x_i(j+1)^T, u_i(j)^T)^T = \tilde{g}, \tag{2.13c}$$

$$\tilde{L}_i (x_i(j+1)^T, u_i(j)^T)^T \leq \tilde{l}_i, \tag{2.13d}$$

$$x_i(k) = x_{i,k}, \tag{2.13e}$$

where N_p stands for the length of a prediction horizon, and $X := (x_1^T,\dots,x_n^T)^T$ and $U := (u_1^T,\dots,u_n^T)^T$ are vectors of state and input variables with the respective reference values denoted using superscript $^{\mathsf{r}}$. Note that the dynamics of the (sub)systems are decoupled and the coupling occurs because of global constraints (2.13c) which might represent limited resources shared among the subsystems or consensus constraints. Hence that the problem (2.13) is straightforwardly condensed into the form (2.1) by expressing the explicit dependency of systems states using the dynamics equations (2.13b).

Here we study a four-tank benchmark [48] whose scheme is shown in Fig. 3. The control task is to track the time-varying references in order to drive the system in the different steady-states.

The cross-sectional areas of all tanks are $S = 0.06\,\mathrm{m}^2$. The considered values of the discharge areas of tank outlets are $a = [1.31 \times 10^{-4}, 1.51 \times 10^{-4}, 9.27 \times 10^{-5}, 8.82 \times 10^{-5}]\,\mathrm{m}^2$ and the distributions ratios of three-way valves are $[\gamma_1, \gamma_2] = [0.3, 0.4]$. Maximum allowed heights of the tanks are $h^{max} = [1.36, 1.36, 1.3, 1.3]\,\mathrm{m}$ for each tank. Pumps of the plant can provide maximum flow rates of $[q_1^{max}, q_2^{max}] = [3.26, 4]\,\mathrm{m}^3/\mathrm{h}$. It is assumed that the liquid levels in tanks are initially set to be at $h^0 = [0.65, 0.66, 0.65, 0.66]\,\mathrm{m}$ that stands for a steady state together which the flow rates $q^0 = [1.63, 2.00]\,\mathrm{m}^3/\mathrm{h}$.

2.2.1 Dynamic Model

The dynamics of the plant can be described as a following set of differential equations

$$\frac{\mathrm{d}h_1}{\mathrm{d}t} = -\frac{a_1}{S}\sqrt{2gh_1} + \frac{a_3}{S}\sqrt{2gh_3} + \frac{\gamma_1}{S}q_1, \tag{2.14a}$$

$$\frac{\mathrm{d}h_2}{\mathrm{d}t} = -\frac{a_2}{S}\sqrt{2gh_2} + \frac{a_4}{S}\sqrt{2gh_4} + \frac{\gamma_2}{S}q_2, \tag{2.14b}$$

$$\frac{\mathrm{d}h_3}{\mathrm{d}t} = -\frac{a_3}{S}\sqrt{2gh_3} + \frac{(1-\gamma_2)}{S}q_2, \tag{2.14c}$$

$$\frac{\mathrm{d}h_4}{\mathrm{d}t} = -\frac{a_4}{S}\sqrt{2gh_4} + \frac{(1-\gamma_1)}{S}q_1. \tag{2.14d}$$

As discussed in [49], this model describes the behavior of the plant reasonably well when the heights in tanks are over $0.2\,\mathrm{m}$. Therefore, the physical lower bounds of the tank heights have been set to $0.2\,\mathrm{m}$. A continuous linear model can be formulated via a linearization of (2.14) around the initial steady state (h^0, q^0) as

$$\frac{\mathrm{d}x}{\mathrm{d}t} = A_c x + B_c u, \tag{2.15a}$$

$$y = C_c x, \tag{2.15b}$$

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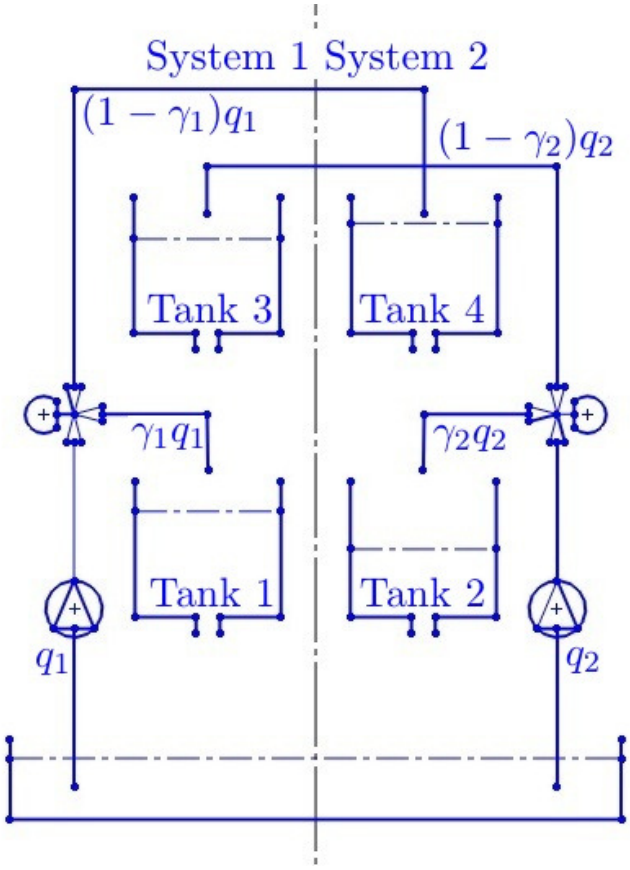

Figure 3: Schematic diagram of a quadruple-tank system.

where $x = (x_1, x_2, x_3, x_4)$ indicate the states variables and $u = (u_1, u_2)$ stand for control inputs, i.e. deviations of the tank levels and flow rates from the steady state (h^0, q^0) of the system. The matrices A_c, B_c and C_c are defined as

$$A_c := \begin{bmatrix} -\mathcal{T}_1 & 0 & \mathcal{T}_3 & 0 \\ 0 & -\mathcal{T}_2 & 0 & \mathcal{T}_4 \\ 0 & 0 & -\mathcal{T}_3 & 0 \\ 0 & 0 & 0 & -\mathcal{T}_4 \end{bmatrix}, \tag{2.16a}$$

$$B_c^T := \begin{bmatrix} \frac{\gamma_1}{S} & 0 & 0 & \frac{1-\gamma_1}{S} \\ 0 & \frac{\gamma_2}{S} & \frac{1-\gamma_2}{S} & 0 \end{bmatrix}, \quad C_c := I, \tag{2.16b}$$

in which $\mathcal{T}_i = a_i/(S\sqrt{2h_i^0/g})$ with $i \in \{1, 2, 3, 4\}$. The discrete-time system is formulated using zero-order hold with sampling time of 90 s.

2.2.2 Control Objective

As in [49], a set of references for heights in the first and the second tank is considered. The overall duration of the control task is 9000 s which is divided into three consecutive intervals of 3000 s with set-points of $h_1^{\mathrm{r}} = \{0.3, 0.5, 0.9\}$ m and $h_2^{\mathrm{r}} = \{0.3, 0.75, 0.75\}$ m. The steady-state flow-rates u_1^{r} and u_2^{r} that correspond to these set-points are calculated according to the nonlinear model of the system.

The centralized model predictive controller minimizes the cost (2.13a) where $N_p = 10$ is the same as the length of a control horizon. The weighting matrices with appropriate dimensions are $Q_{x,i} = I$ and $Q_{u,i} = 0.01\, I$. Note that the stability of MPC is out of the scope of this work, thus, we do not impose terminal-cost term into the objective which generally results in a non-decomposable objective.

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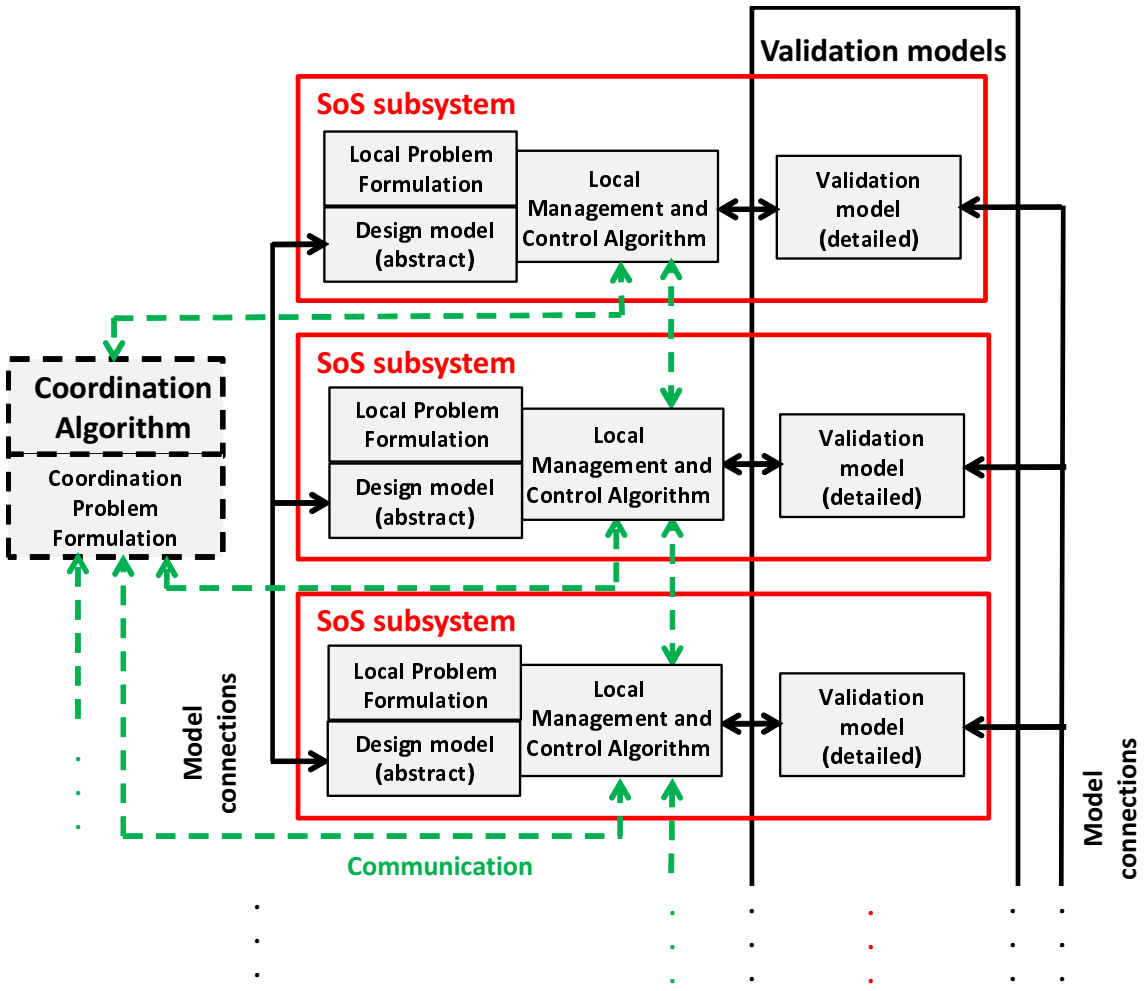

Figure 4: The structure of a controlled system in the simulation and validation framework.

A distributed MPC scheme is realized such that the system is decomposed into two subsystems, one concerned with the heights in the first and the third tank and the other one concerned with the heights in the second and the fourth tank. Therefore, the states in these subsystems are:

$$x_{s1} = (x_1, x_3)^T, \quad x_{s2} = (x_2, x_4)^T. \tag{2.17}$$

Upon observing (2.15), it is clear that this decomposition leaves no state couplings to be present. On the other hand, both subsystems are given the freedom to adjust (optimize) the flow-rates q_1 and q_2 which gives rise to the notion of shared resources, i.e. input couplings, as the global (overall) system optimum requires

$$q_i^1(j) = q_i^2(j), \quad i = 1, 2,\ j \in \{k, \ldots, k + N_p - 1\}, \tag{2.18}$$

where the superscript assigns the decision to the respective subsystem.

2.3 Implementation and Results

We use the Modeling, Simulation and Validation Framework (MSVF) developed in the WP 4 of the DYMASOS project for the implementation of the distributed MPC. We implement here the controllers of the particular subsystems and the dynamic management realized via a coordination principle described in the previous section.

Figure 4 represents the general structure of a controlled system which is implemented within the MSVF. It is necessary to point out that the design models and the local and global problem formulations are not implemented as individual

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components within the framework and are considered as a part of the local controllers and the global coordinator. The MSVF provides standardized interfaces to which the management algorithms and models can be easily connected. Such standard interfaces also provide a straightforward avenue for the deployment of management solutions to industrial hardware systems at a later stage.

The main implementation focuses of the framework, its main components as well as the generic Modelica-based interfaces are reported in detail in deliverables D4.1 and D4.2 of the DYMASOS project.

As shown in D4.2., the fact that the Modelica language is chosen as the base implementation language of the framework, does not mean that the modeling language is restricted to Modelica, as such; the controller components of the four-tank benchmark are implemented in MATLAB. To connect these components to the MSVF, C-based shared libraries were created using the MATLAB compiler [50].

2.3.1 Using the MATLAB Compiler

The MATLAB compiler [50] enables the user to create standalone C and C++ applications on Unix, Windows and Mac as well as C and C++ shared libraries (Dynamic Link Libraries (.dll) and .so on Windows and Linux platforms respectively) from M-files, MEX-files or other MATLAB-based code. It supports the full MATLAB language as well as most of the toolboxes and user-developed user interfaces. The MATLAB compiler also creates platform-specific *wrapper* files which provide an interface to the compiled MATLAB code. These files define the data arrays that are used by the compiled code, provide the required routines to "forward calls from interface functions to the MATLAB functions in the complier runtime" [50].

Shared libraries can share an instance of the Matlab Compiler Runtime (MCR) as long as the instance is initialized and terminated correctly. For the initialization of the MCR instance, the functions `mclInitializeApplication` and `mclmcrInitialize` have to be called once in the beginning of the application before any other call to MATLAB functions to generate and set global options of the instance and setting the environment for calling MATLAB functions. The termination routine has to be called only at the end of the application where all the MCR instances have been destroyed using the `mclTerminateApplication` function. One has to keep in mind that after termination no MATLAB function can be called and the MCR cannot be initialized again. Also, initializing the MCR instance more than once will cause the program not to function properly.

2.3.2 The DLL Interface

Based on the aforementioned information, a generic interface that can communicate with C shared libraries was developed. The choice of C is supported by the fact that the calls to external C or Fortran functions are supported by Modelica platforms. The design of the interface was inspired by MATLAB S-function interface in which the simulation information is passed as a structure to a number of callback methods [51]. For more details on the implementation of the DLL interface, the reader is referred to the deliverable D4.4 of the DYMASOS project.

2.3.3 Implementation

As mentioned earlier, the controller components of the demonstration example are implemented in MATLAB and were compiled using the MATLAB compiler and connected to the framework as black-box components using the DLL interface. The generic interfaces were parametrized based on the information that is shared between the local optimization problems and the coordinator namely the price vector λ from the coordinator and the responses q_i from the local optimization problems. The iterations between the components are implemented through the event interfaces which ensures a deterministic order of execution. The implementation details of the event interfaces is also explained in detail in D4.4. The generation of the communication structure is done manually for this particular example.

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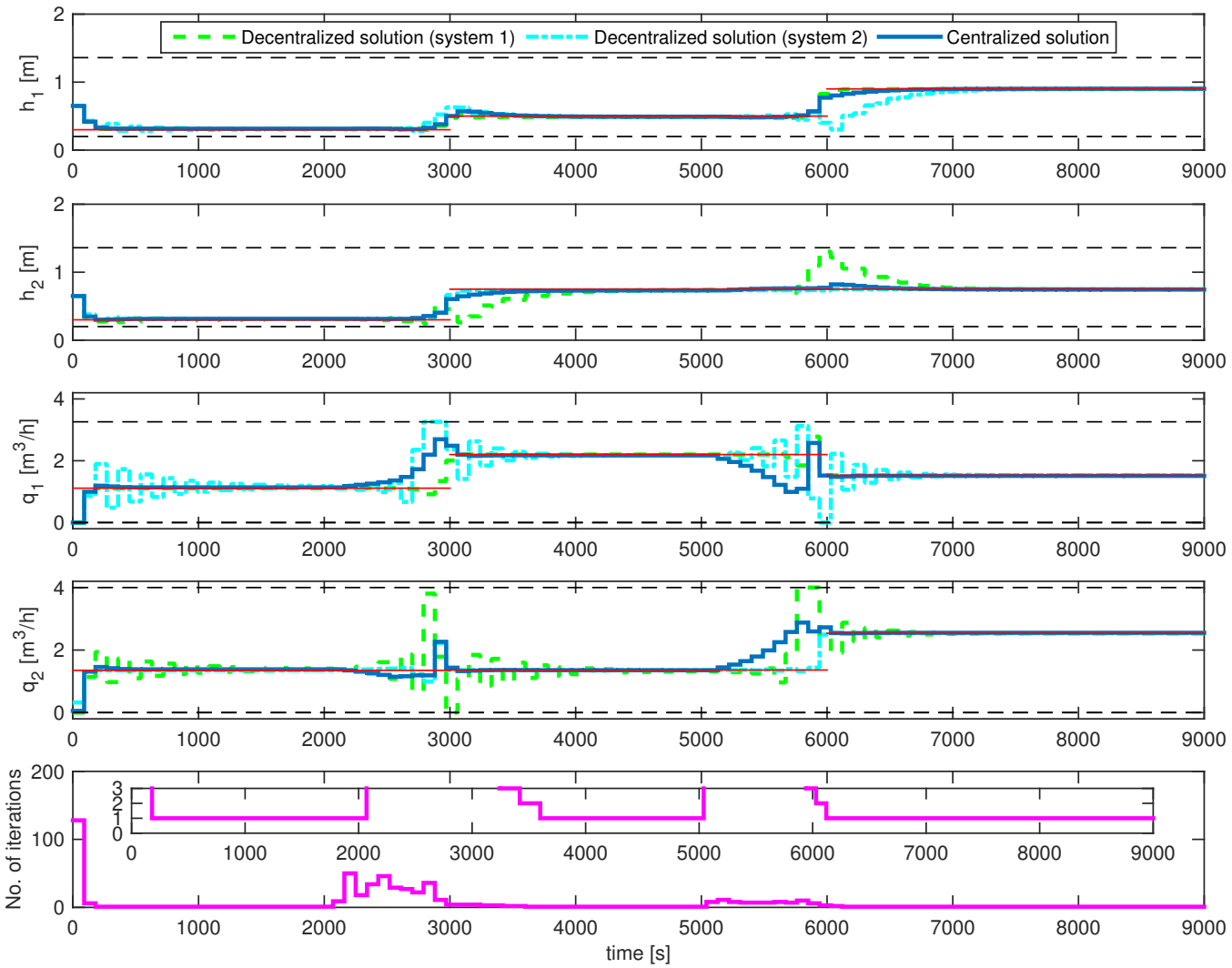

Figure 5: Comparison of the simulation results obtained for centralized and decentralized control schemes. The references are plotted using red solid lines. Constraints are shown with dashed lines. The lower plot shows the number of iterations required for price-based coordination scheme to converge.

2.3.4 Simulation Results

The simulation and validation framework implements validation (nonlinear) models in Modelica while the design (linearized) models of the local controllers and the global coordinator are implemented in MATLAB using YALMIP toolbox [52] and are compiled as DLLs which are connected to the framework using the DLL interface.

Figure 5 shows the results obtained for the different control schemes: centralized and decentralized with subsystem 1 (respectively subsystem 2) assign the degrees of freedom. The decentralized solution, when the system 1 (respectively system 2) optimizes its own objective function and applies the resulting local optimal control policy, results in a 2.7-fold, respectively 1.8-fold, deterioration of the global performance.

The distributed MPC coordinated by price-based mechanism achieves the same performance as centralized optimization. It is also able to tackle the situations where the local constraints are active (e.g. at times 0 s and 2,600 s the lower limit is hit for the flow-rate q_1 and height in the third tank respectively) but this is achieved, as might be expected, for the price of increased number of iterations. This behavior is attributed to the subgradient update which is able to maintain ratios of elements of vector λ close to optimum. Hence when the local constraints are inactive (over the whole prediction horizon) a single iteration is required for the coordinator to adjust the price vector to the equilibrium value.

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3. Extensions of Market-based Coordination for Continuous Production Units

In this section a hierarchical shared resource allocation problem is revisited. This problem originates from management structure of an industrial production complex as shown in Fig. 2 and as studied in the INEOS case study of the DYMASOS project. First, a novel price-update strategy is presented that relies on quadratic approximation of the residual of network balance. Then the market-like mechanism based on Alternating Direction Method of Multipliers (ADMM) is presented that extends the applicability of the price-based coordination to problems with non-strictly convex local objective functions and problems with strong involvement of local constraints.

3.1 Novel Price-update Strategy Using Quadratic Approximation

The general subgradient-based update law of price coordinator (2.9), as discussed in the previous section, involves a degree of freedom, which is the choice of the step size parameter α^k. The parameter has a strong influence on the performance and convergence properties of the approach and can lead to divergence of the scheme, if not properly chosen. An extensive discussion about convergence rates and different approaches to choose α^k can be found for example in [53]. Common choices are, for instance, a fixed step length or a decreasing step size, which is chosen off-line a priori to the coordination run. In a ideal case, when the dual function is differentiable, the local constraints of the subsystems do not play a big role and the coordinator is able to access the information about the structure of the local problems, this parameter can be chosen using the expression (2.12). In general case a coordinator can build a surrogate model of the gradients or Hessians of the local plants objectives. This approach was pursued in [54, 55, 56, 57]. Here we present our recently developed approach [56], which gives a a novel way to find the equilibrium price, while maintaining the confidentiality features of the price-based coordination.

3.1.1 Modeling the Optimal Resource Allocation as a QP

For the following derivation we assume that the site-wide optimization problem can be formulated as cooperative resource allocation problem around the feasible operating point of the complex with quadratic cost functions. The resulting formulation is (2.1). The underlying assumptions are valid, since a typical cost function contains linear economic contributions as well as quadratic tracking terms to fulfill certain production rates (e.g., set in internal contracts).

In the following, the model of a plant i is formulated as a linear mapping from the inputs to the states:

$$x_i = M_{ux,i} u_i + V_{x,i}, \tag{3.1}$$

where the matrix $M_{ux,i} \in \mathbb{R}^{n_{x_i} \times m_i}$ links the inputs to the states and $V_{x,i} \in \mathbb{R}^{n_{x,i}}$ defines a constant offset of the model. The product vector y_i is a subset of the states and is computed by the following relation:

$$y_i = M_{xy,i} x_i, \tag{3.2}$$

with the matrix $M_{xy,i} \in \mathbb{R}^{n_{y_i} \times n_{x_i}}$. The shared resource vector is a combination of contributions from the inputs as well as from the products (states). Hence the utilization vector can be written as the linear combination:

$$R_i = M_{xR,i} x_i + M_{uR,i} u_i, \tag{3.3}$$

with $M_{uR,i} \in \mathbb{R}^{g \times m_i}$ and $M_{xR,i} \in \mathbb{R}^{n_R \times n_{x_i}}$. As previously mentioned, the sign of an entry in R_i decides whether a resource is consumed or produced. If the plant is not connected to a respective network the entry is set to zero.

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The underlying mathematical optimization problem can then be formulated as

$$\min_{u_i\ \forall i} \sum_{i=1}^{n} \frac{1}{2} y_i^T P_i y_i + \frac{1}{2} u_i^T \tilde{H}_i u_i + p_i^T y_i + \tilde{w}_i^T u_i \tag{3.4a}$$

$$\text{s.t. } M_{xy,i} x_i = y_i, \tag{3.4b}$$

$$M_{ux,i} u_i + V_{x,i} = x_i, \tag{3.4c}$$

$$M_{xR,i} x_i + M_{uR,i} u_i = R_i(x_i, u_i), \tag{3.4d}$$

$$\sum_{i=1}^{n} R_i(x_i, u_i) + R_e = 0, \tag{3.4e}$$

where the tracking term matrices $P_i \in \mathbb{R}^{n_{y_i} \times n_{y_i}}$ and $\tilde{H}_i \in \mathbb{R}^{m_i \times m_i}$ are symmetric and positive definite ($P_i,\ \tilde{H}_i \succ 0$). The relations (3.4b)–(3.4d) contain the stationary model equations of the plants, where $x_i \in \mathbb{R}^{n_{x_i}}$ are the states of plant i and $y_i \in \mathbb{R}^{n_{y_i}}$ are the products. The constraint (3.4e) is the global network balance, where $R_e \in \mathbb{R}^{n_R}$ is the offset that incorporates fixed resource flows over the boundaries of the production complex.

The problem (3.4) can be reformulated in a compact form with u_i as manipulated variables, since the states and products are affine functions

$$\min_{u_i\ \forall i} \sum_{i=1}^{n} \frac{1}{2} u_i^T H_i u_i + w_i^T u_i \tag{3.5a}$$

$$\text{s.t. } \sum_{i=1}^{n} R_i(u_i) + R_e = \sum_{i=1}^{n} G_i u_i = g, \tag{3.5b}$$

where the H_i and w_i are the following lumped linear combinations

$$H_i = \tilde{H}_i + M_{ux,i}^T M_{xy,i}^T P_i M_{xy,i} M_{ux,i}, \tag{3.6a}$$

$$w_i^T = \tilde{w}_i^T + \left(V_{x,i}^T M_{xy,i}^T P_i + p_i^T\right) M_{xy,i} M_{ux,i}, \tag{3.6b}$$

$$G_i = M_{xR,i} M_{ux,i} + M_{uR,i}. \tag{3.6c}$$

With the above mentioned assumption the local decisions of a plant i can be expressed as

$$u_i^* = -H_i^{-1} \left(w_i + G_i^T \lambda\right). \tag{3.7}$$

3.1.2 Establishing a Link between the Subgradient and the Lagrange Multipliers

Practical resource allocation problems often require a high number of iterations for the price-based coordination algorithm to converge. Thus, it is tried to find a new update strategy that finds the equilibrium price with few iterations. For the optimization problem shown in (3.4) a link can be established between the prices and the residual of the network balance [56].

Taking the squared two-norm of the global constraint yields:

$$\left\| \sum_{i=1}^{n} G_i u_i^*(\lambda) - g \right\|_2^2 = \left(\sum_{i=1}^{n} G_i u_i^*(\lambda) - g \right)^T \left(\sum_{i=1}^{n} G_i u_i^*(\lambda) - g \right). \tag{3.8}$$

Introducing the solution for the optimal local decisions:

$$\left(\sum_{i=1}^{n} G_i u_i^*(\lambda) - g \right)^T \left(\sum_{i=1}^{n} G_i u_i^*(\lambda) - g \right) =$$

$$\left(\sum_{i=1}^{n} G_i \left(-H_i^{-1} \left(w_i + G_i^T \lambda\right)\right) - g \right)^T \left(\sum_{i=1}^{n} G_i \left(-H_i^{-1} \left(w_i + G_i^T \lambda\right)\right) - g \right) = \ldots \tag{3.9}$$

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Expanding the expression

$$\ldots = \left(\left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right)^T + \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right)^T + \left(\sum_{i=1}^{n} g\right)^T\right) \left(\left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right) + \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right) - \left(\sum_{i=1}^{n} g\right)\right) = \ldots \quad (3.10)$$

Multiplying the single terms yields

$$\begin{aligned}\ldots = &\left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right) + \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right) \\ &- \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right)^T \left(\sum_{i=1}^{n} g\right) + \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right) \\ &+ \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right) - \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right)^T \left(\sum_{i=1}^{n} g\right) \\ &- \left(\sum_{i=1}^{n} g\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right) - \left(\sum_{i=1}^{n} g\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right) \\ &+ \left(\sum_{i=1}^{n} g\right)^T \left(\sum_{i=1}^{n} g\right). \end{aligned} \quad (3.11)$$

The expanded expression contains constant, linear and quadratic terms. Thus, it can be written in the compact form below

$$f_r(\lambda) = \left\| \sum_{i=1}^{n} G_i u_i^* - g \right\|_2^2 = \lambda^T S \lambda + h^T \lambda + k, \quad (3.12)$$

where the variables S, h and k can be inferred by collecting the respective terms. First, collecting the constants from (3.11):

$$\begin{aligned} k = &\left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right) + \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right)^T \left(\sum_{i=1}^{n} g\right) \\ &- \left(\sum_{i=1}^{n} g\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right) + \left(\sum_{i=1}^{n} g\right)^T \left(\sum_{i=1}^{n} g\right). \end{aligned} \quad (3.13)$$

Since the bracket contain vectors ($a^T b = b^T a$) the expression can be rewritten as

$$k = \left(\sum_{i=1}^{n} w_i^T H_i^{-1} G_i^T\right) \left(\sum_{i=1}^{n} G_i H_i^{-1} w_i + 2g\right) + \left(\sum_{i=1}^{n} g\right)^T \left(\sum_{i=1}^{n} g\right). \quad (3.14)$$

Second, collecting the linear terms from (3.11) ($a^T b = b^T a$):

$$\begin{aligned} h^T \lambda = &\left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right) + \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} w_i\right) \\ &- \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right)^T \left(\sum_{i=1}^{n} g\right) - \left(\sum_{i=1}^{n} g\right)^T \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T \lambda\right) = \\ &2 \left(\left(\sum_{i=1}^{n} G_i H_i^{-1} w_i\right)^T + \left(\sum_{i=1}^{n} g\right)^T\right) \left(\sum_{i=1}^{n} G_i H_i^{-1} G_i^T \lambda\right). \end{aligned} \quad (3.15)$$

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Further simplification yields

$$h^T = 2\left(\sum_{i=1}^{n} w_i^T H_i^{-1} G_i^T + g^T\right)\left(\sum_{i=1}^{n} G_i H_i^{-1} G_i^T\right). \tag{3.16}$$

The remaining term in (3.11) represents the quadratic contribution

$$\lambda^T S\lambda = \left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T\lambda\right)^T\left(\sum_{i=1}^{n} -G_i H_i^{-1} G_i^T\lambda\right) = \left(\sum_{i=1}^{n} \lambda^T\left(G_i H_i^{-1} G_i^T\right)^T\right)\left(\sum_{i=1}^{n} G_i H_i^{-1} G_i^T\lambda\right) = \left(\sum_{i=1}^{n} \lambda^T G_i H_i^{-1} G_i^T\right)\left(\sum_{i=1}^{n} G_i H_i^{-1} G_i^T\lambda\right). \tag{3.17}$$

Thus the matrix S is defined as

$$S = \left(\sum_{i=1}^{n} G_i H_i^{-1} G_i^T\right)\left(\sum_{i=1}^{n} G_i H_i^{-1} G_i^T\right). \tag{3.18}$$

Finally, the relation can be expressed as

$$f_r(\lambda) = \left\|\sum_{i=1}^{n} G_i u_i^* + g\right\|_2^2 = \lambda^T S\lambda + h^T\lambda + k. \tag{3.19}$$

3.1.3 Formulation of the Algorithm

The goal of the proposed strategy is to make use of the derived relation to find the equilibrium price with few iterations. If the variables $S \in \mathbb{R}^{n_R \times n_R}$, $h \in \mathbb{R}^{n_R}$ and $k \in \mathbb{R}$ were available, the function $f_r(\lambda)$ would be known and the equilibrium price could be determined. In practice however this is rarely the case due to the aforementioned reasons. Consequently, these variables have to be determined based on limited knowledge. One possibility is to determine the necessary information by probing the subsystems with a sufficient amount of price vectors and "measuring" the response, i.e. the residual of the network balance. The minimum number of price vectors depends on the number of shared resources and is independent of the number of subsystems:

$$n_{QA,min} = \frac{(n_R+1)(n_R+2)}{2}, \tag{3.20}$$

with n_R being the number of shared resources. When enough points are collected, S, h and k can be determined by interpolation. The procedure is inspired by derivative-free optimization methods that employ surrogate models of sampled function values in the absence of derivatives [58].

In order to successfully build such a surrogate model—in this case a quadratic model is considered—a reasonable set of interpolation points has to be collected. The points selected for the approximation of the quadratic function have to contain a sufficient amount of information about the curvature of the underlying problem. It has to be ensured that a minimum of $n_{QA,min}$ points is choses that are linearly independent. Otherwise the approximation fails. Another critical point is the assumption made on the locally unconstrained plants. In most technical applications it is questionable whether the underlying problem is unconstrained and the derived relations hold.

In [59] an algorithm has been proposed that selects a suitable set of points for a robust and reliable approximation. Although, the algorithm therein was developed for a different application, it serves well the purpose considered here. Using the relation derived for $f_r(\lambda)$ the price update step can be replaced by:

$$\lambda^{k+1} = \underset{\lambda\in\Lambda^k}{\arg\min}\ f_r^k(\lambda), \tag{3.21}$$

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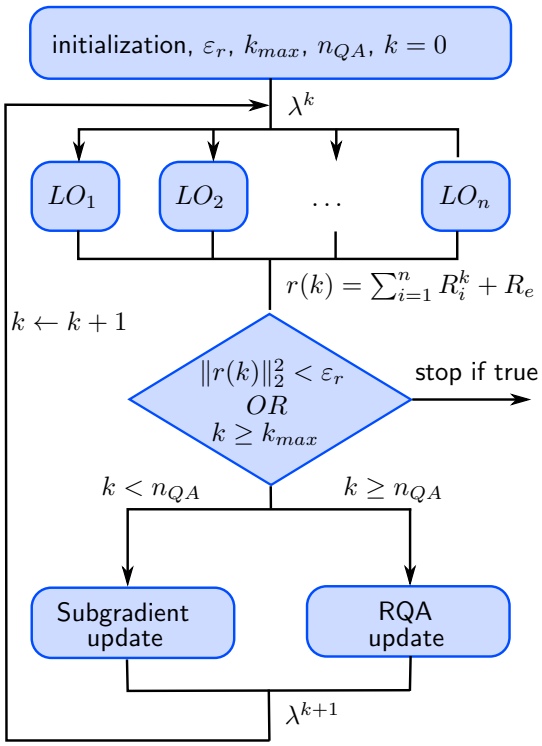

Figure 6: Block diagram of the novel coordination procedure.

where f_r^k is the quadratic function fitted in step k to the selected point sets $(\mathcal{S}_{f_r}, \mathcal{S}_\lambda)$ containing the probed price vectors and responses and Λ^k is a limited search space for the next price vector (e.g., in the simplest case a box constraint).

The strategy applied to solve the optimal resource allocation problem is depicted in Fig. 6. After initializing the algorithm with the necessary settings (e.g., maximum number of iterations, tolerances and update-specific settings), the first set of required points is attained by using subgradient updates. The initial price is sent by the coordinator to the local optimizers ($LO_i \; \forall i$), which solve their local optimization problems and respond with a shared resource utilization. The responses are collected by the coordinator and the residual is evaluated. If the convergence criterion is not met, the prices are updated using subgradient updates until n_{QA} points are collected. Here, n_{QA} is at least the number of points that is needed to fit a quadratic function $n_{QA,min}$, but can be chosen to be higher to collect more initial data before the startup of the approximation. After enough points have been collected, the sets $(\mathcal{S}_{f_r}^k, \mathcal{S}_\lambda^k)$ of points are constructed to fit the quadratic function f_r^k. The next price is found by minimizing the function according to (3.21). In most of the cases the first quadratic approximation will not result in the equilibrium price, since the collected set of points by subgradients updates might incorporate linear dependent price vectors, leading to a not well-poised set of interpolation points. Consequently, the algorithm has to be run iteratively and is referred to as recursive quadratic approximation (RQA). In this recursive strategy the responses of the local optimizers with respect to the new prices are included in the next quadratic approximation and $(\mathcal{S}_{f_r}, \mathcal{S}_\lambda)$ are updated to construct the next quadratic approximation until convergence is achieved.

3.1.4 Demonstration Examples

In this section we present two case studies of different complexity. First, an artificial resource allocation problem that consists of three locally unconstrained production plants and two utility networks is formulated. Secondly, a case study is presented that is based on a simplified version of the steam network at INEOS in Köln as described by [5].

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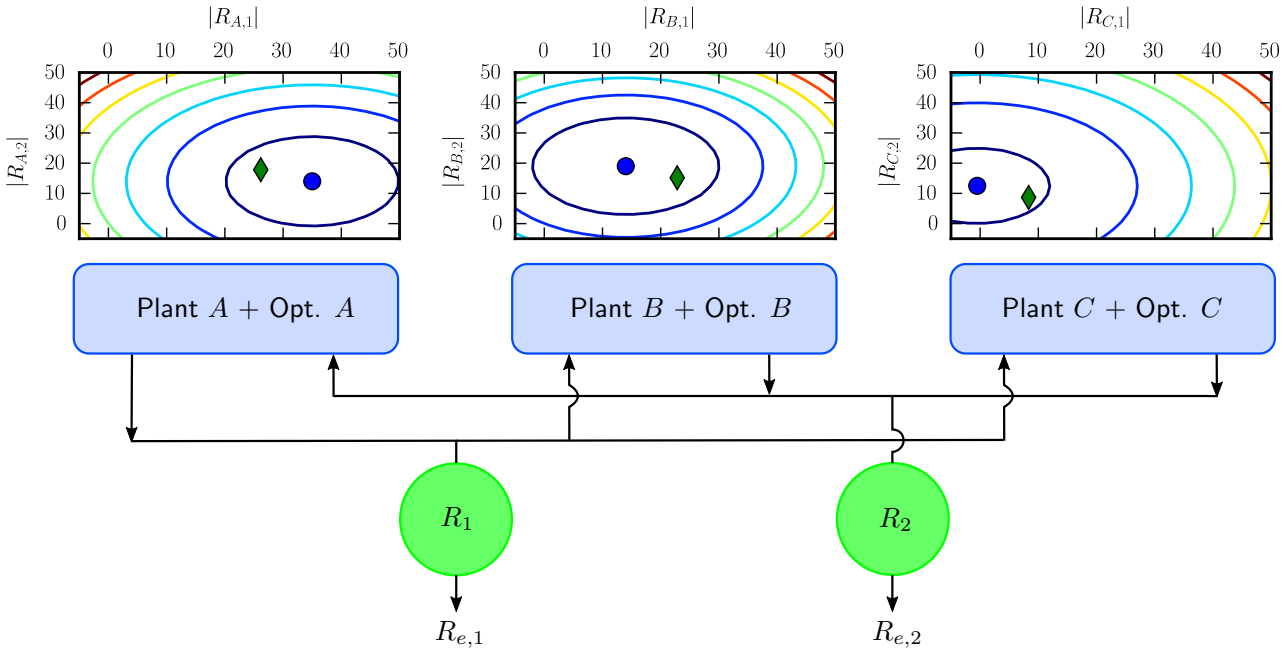

Figure 7: Case study consisting of three plants with unconstrained local quadratic cost functions. Two resources (R_1 and R_2) are shared among the plants. Additionally, two export streams $R_{e,i}$ and $R_{e,2}$ leave the networks, which have fixed values. In the contour plots the dots indicate the uncoordinated optima of the plants (i.e., optimal in respect to the local cost function, but not respecting the global constraint), while the diamonds show the optimal local resource utilization the fulfills the global constraint.

Coordination of Locally Unconstrained Production Plants

We consider three locally unconstrained production plants with local optimizers as shown in Fig. 7. The local cost functions are quadratic programs that incorporate linear economic and quadratic tracking terms, which result from casting the production demand reference into an input tracking problem. The local cost functions have the following generic form

$$J_i(u_i) = \underbrace{p_{i,1} \cdot u_{i,1} + p_{i,2} \cdot u_{i,2}}_{\text{sales and raw material costs}} + \underbrace{(u_{i,1,ref} - u_{i,1})^2 + (u_{i,2,ref} - u_{i,2})^2}_{\text{input tracking}}, \; i \in [A,\, B,\, C], \tag{3.23}$$

where $u_i \in \mathbb{R}^2$ contains the manipulated variables, $u_{i,j,ref}$ are references and $p_{i,j}$ are the prices that are assigned to bought or sold quantities, i.e., produced and consumed shared resources.

Table 1: Model parameters for the coordination of three unconstrained quadratic subsystems. Negative prices denote sales prices.

	$p_{i,1}$	$p_{i,2}$	$u_{i,1,ref.}$	$u_{i,2,ref.}$
Plant A	-10	8	30	18
Plant B	12	-14	20	12
Plant C	11	-13	5	6

$$\begin{gathered} R_e = \begin{pmatrix} -5 & -6 \end{pmatrix}^T, \quad M_{uR,1} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad M_{uR,2} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ M_{uR,3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad H_i = 2 \cdot I, \quad w_i = \begin{pmatrix} p_{i,1} - 2u_{i,1,ref} \\ p_{i,2} - 2u_{i,2,ref} \end{pmatrix}. \end{gathered} \tag{3.22}$$

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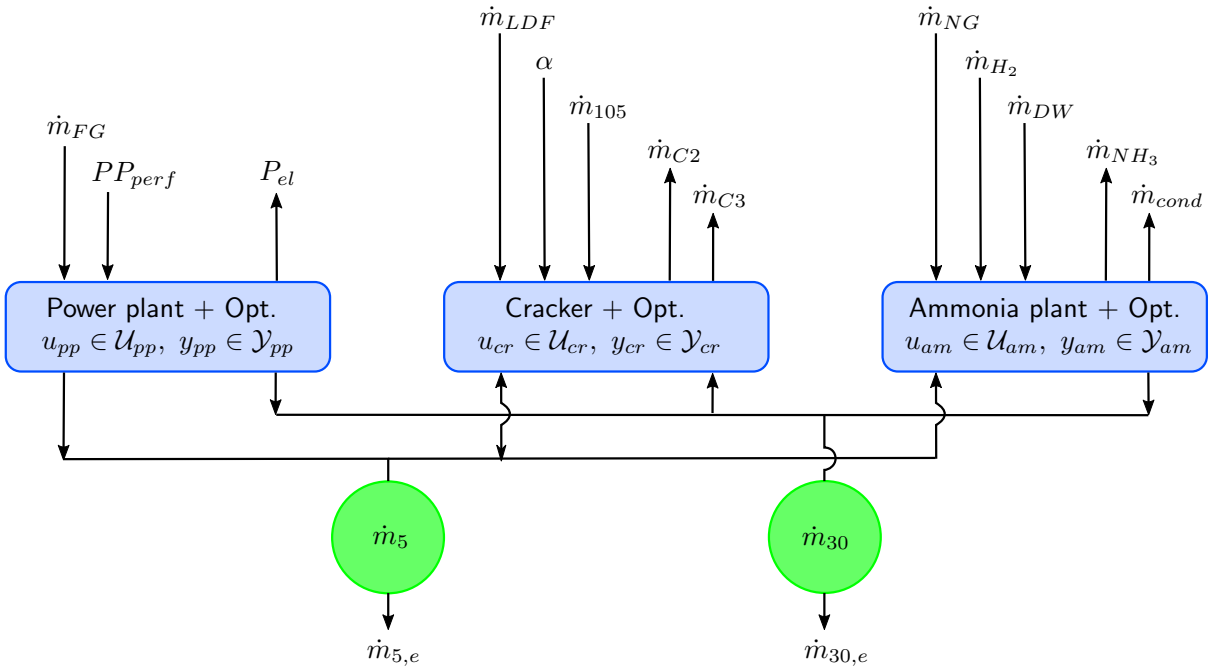

Figure 8: Case study consisting of three locally constrained plants, namely a power plant, a cracker, and an ammonia plant. The three plants are connected by the 5 bar and 30 bar networks.

Following the formulation of the optimization problem (3.4) and the expression for the shared resources, the optimal resource allocation problem for the three quadratic subsystems can be written as

$$\min_{u_i\ \forall i} \sum_{i=1}^{n} \frac{1}{2} u_i^T H_i u_i + w_i^T u_i \tag{3.24a}$$

$$\text{s.t.} \sum_{i=1}^{n} R_i + R_e = 0, \tag{3.24b}$$

$$R_i = M_{uR,i} u_i, \tag{3.24c}$$

where $R_e \in \mathbb{R}^2$ denotes the vector of exported quantities. The model parameters are given in Table 1. The centralized formulation of the optimization problem can be distributed and thus the following local Lagrangian functions can be defined

$$\mathcal{L}_i(u_i, \lambda) = \frac{1}{2} u_i^T H_i u_i + (w_i^T + \lambda^T M_{uR,i}) u_i, \tag{3.25}$$

with the optimal resource utilization of subsystem i as a function of the transfer price vector λ

$$R_i(\lambda) = M_{uR,i} \ \arg\min_{u_i} \mathcal{L}_i(u_i, \lambda) = -M_{uR,i} H_i^{-1} (w_i + M_{uR,i} \lambda). \tag{3.26}$$

Steam Management in a Petrochemical Production Site - INEOS Case Study

This case study is based on a simplified model of the highly integrated petrochemical production site of INEOS in Köln as described by [5].

The resource allocation problem comprises a power plant, a cracker, and an ammonia plant that share steams at different pressure levels via two shared resource networks, the 5 bar and the 30 bar steam network as illustrated in Fig. 8. The structure of the case study is comparable with the coordination case of three unconstrained production plants (see section 3.1.4). However, the local plants in the industrial case study are constrained by local limits (3.27e) on input (manipulated) variables and outputs. These local limits are due to operational constraints of the equipment,

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safety considerations and contracts with customers or producers on the site. Additionally, the set of input and output variables is different from the set of shared resource variables. In the following a brief description of the single plants is given.

The main purpose of the power plant is to burn off gases of adjacent production processes on site or fuel gas in order to produce electricity and steam on two different pressure levels needed by the industrial complex. The manipulated variables considered here are the fuel gas consumption $\dot{m}_{FG}$ and the power plant performance factor PP_{perf}, which determines the ratio of the two steam levels produced by the plant. The electrical power is considered as a product that can be sold, while the two steam flows are sent to the shared resource networks for 5 bar and 30 bar.

The cracker represents the heart of the petrochemical production site. The incoming naphtha stream $\dot{m}_{LDF}$ is cracked in order to produce different petrochemical intermediates such as the main products ethylene $\dot{m}_{C2}$ and propylene $\dot{m}_{C3}$ that are considered here. In addition to the input of naphtha, the severity of the cracker α (i.e., the ratio of C2/C3) and the input stream of an additional 105 bar steam can be manipulated.

In the ammonia plant, hydrogen and fuel gas are used to produce ammonia, the main product of this plant. The manipulated variables are the natural gas intake $\dot{m}_{NG}$, the hydrogen intake $\dot{m}_{H_2}$ and the deionized water consumption $\dot{m}_{DW}$. The plant uses steam from the 5 bar network and produces 30 bar steam.

Since the local constraints on inputs and products are partially nonlinear, we consider the following notation. If the network balance is neglected, the plants (power plant, cracker, ammonia plant) solve the following local optimization problem in parallel in a distributed fashion

$$\min_{u_i} J_i(u_i) = \min_{u_i} \frac{1}{2} y_i^T P_i y_i + \frac{1}{2} u_i^T \tilde{H}_i u_i + p_i^T y_i + \tilde{w}_i^T u_i \tag{3.27a}$$

$$\text{s.t. } M_{xy,i} x_i = y_i, \tag{3.27b}$$

$$M_{ux,i} u_i + V_{x,i} = x_i, \tag{3.27c}$$

$$M_{xR,i} x_i + M_{uR,i} u_i = R_i(x_i, u_i), \tag{3.27d}$$

$$u_i \in \mathcal{U}_i,\ y_i \in \mathcal{Y}_i, \tag{3.27e}$$

where (3.27b) and (3.27c) are the model equations and (3.27e) represents the local constraints on input and product variables. For the sake of clarity (3.27)), comprising all model equations and constraints, will be abbreviated as $\tilde{f}_i(u_i)$. The optimization problem that has to be solved for the overall production complex includes the global constraint of balanced networks.

$$\min_{u_i,\, \forall i} \sum_{i=1}^{n} J_i(u_i) \tag{3.28a}$$

$$\text{s.t. } \sum_{i=1}^{n} R_i(u_i) + R_e = 0. \tag{3.28b}$$

By Lagrangian relaxation the global constraint is introduced into the objective function and a separable Lagrangian function can be defined

$$\mathcal{L}(U, \lambda) = \sum_{i=1}^{n} J_i(u_i) + \lambda^T \sum_{i=1}^{n} R_i(u_i), \tag{3.29}$$

where the exported or imported quantities R_e can be neglected, since they are constant. The optimal shared resource utilization of a local plant for a given price vector λ can then be formulated as

$$R_i(\lambda) = M_{uR,i} \arg\min_{u_i} \mathcal{L}_i(u_i, \lambda). \tag{3.30}$$

3.1.5 Implementation and Results

In the following section, results for the simulation of the two described case studies are provided. For both case studies price-based coordination is applied, comparing the classical subgradient update with the novel approach of recursive quadratic approximation (RQA) described in section 3.1.

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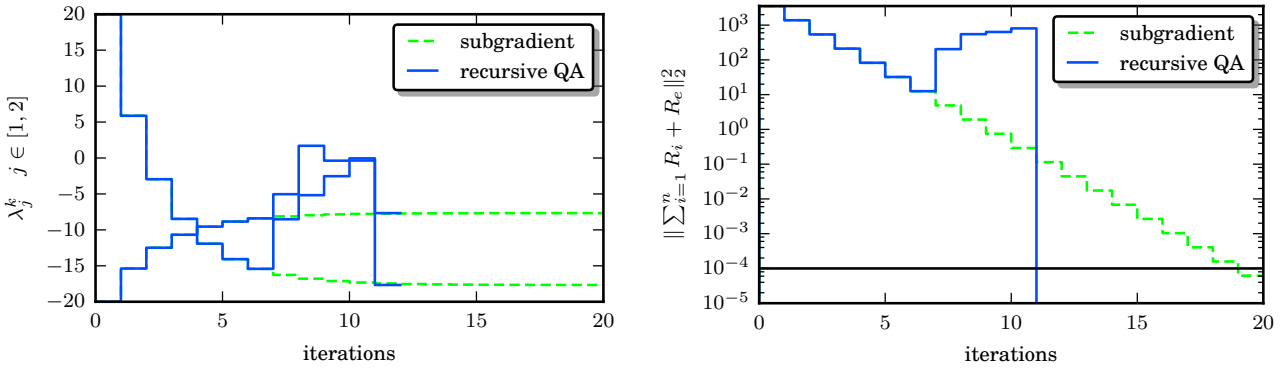
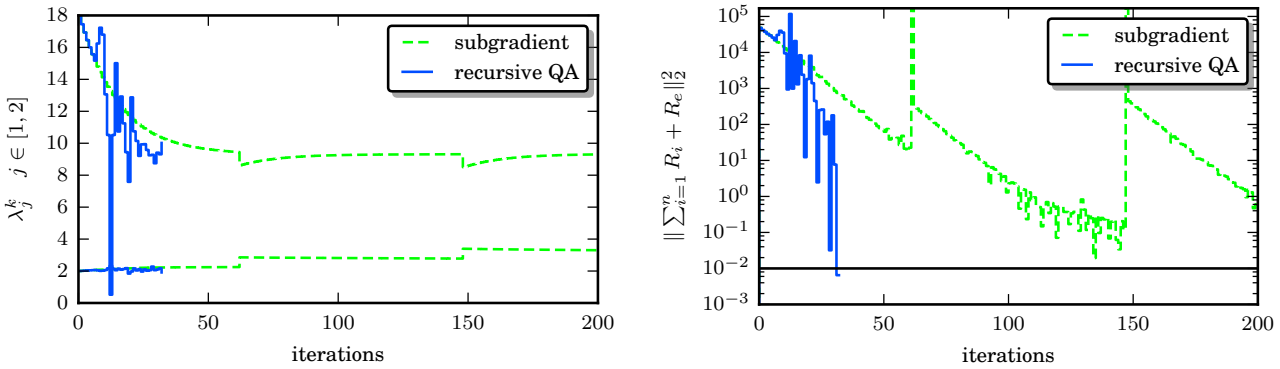


a) Evolution of the prices ($\lambda_1^0 = 20$, $\lambda_2^0 = -20$). b) Evolution of the network balance.

Figure 9: Simulation results for the coordination of three locally unconstrained production plants.



a) Evolution of the prices ($\lambda_1^0 = 18$, $\lambda_2^0 = 2$). b) Evolution of the network balance.

Figure 10: Simulation results for the coordination of three production plants with local constraints of the petrochemical production site of INEOS in Köln.

In addition to the evolution of the price-vectors λ^k and the squared 2-norms of the network residual versus the number of iterations, an analysis of the response surfaces of the network residual as a function of the price vector is done. The resulting heat plots provide insight into some situations in which price-based coordination encounters difficulties.

Results for the Coordination of Locally Unconstrained Production Plants

For the coordination of three unconstrained subsystems the simulation results are shown in Fig. 9. The dashed lines show the evolution of the subgradient update (2.9) for a fixed parameter $\alpha^k = 0.25$ (shows fast, non oscillatory convergence) and a termination tolerance of $\varepsilon_r = 10^{-4}$. It can be seen that after approximately ten iterations the prices are already near the optimal price. However, it takes another ten iterations to converge, since the residual is decreasing linearly.

The RQA starts after six iterations, resulting first in updated prices that worsen the network balance. Nevertheless, it can be observed that after these few iterations the RQA converges exactly to the optimal price vector. The movement in the λ-space can be interpreted as exploration phase in which the algorithm collects necessary information on the network mapping.

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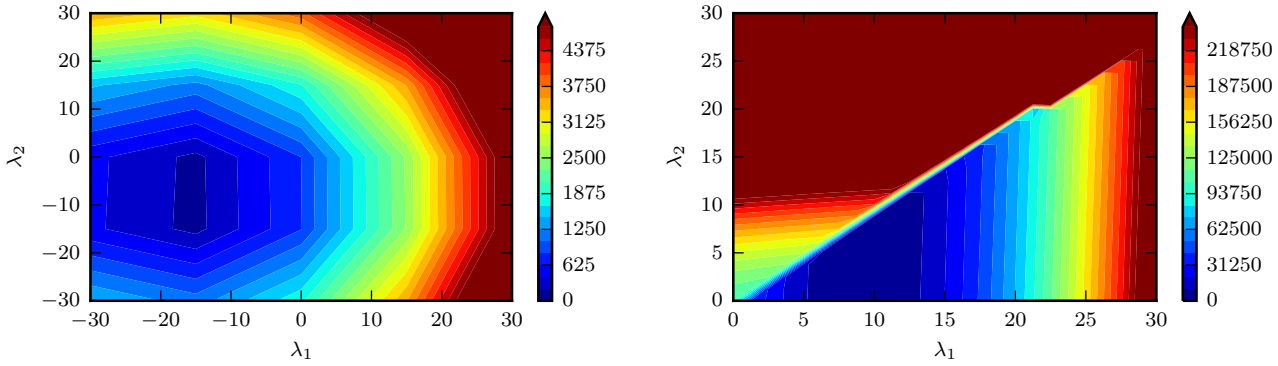

a) Three quadratic subsystems.

b) INEOS in Köln case study.

Figure 11: Response surfaces of the network residual for both case studies as function of the price vector λ.

Results for the Steam Management in a Petrochemical Production Site - INEOS Case Study

The industrial case study of three locally constrained production plants shows a higher sensitivity to transfer prices in comparison to the locally unconstrained plants. Consequently, the price update parameter α^k is chosen to be $2.5 \cdot 10^{-3}$ (higher values have shown diverging behavior) and the termination tolerance of the squared 2-norm of the residual of the network ε_r is set to 10^{-2}, which is a reasonable value for the technical system at hand. The allowed price change constraint for the RQA is set to $\Lambda^k = \|\lambda^{k+1} - \lambda^k\|_2 < 10.0$ (see (3.21)). The simulation results are shown in Fig. 10. It can be noticed that the subgradient-based update improves the network balance from the initial point on, but there are jumps in the prices around iteration 60 and 145. This behavior is caused by local constraints of the subsystems that are not visible to the coordinator, influencing the mapping significantly (see the analysis in the next section). After the jumps, the subgradient-based prices recover and slowly improve the network balance towards the termination tolerance. Within the $k_{max} = 200$ iterations the subgradient-based is not able to balance the networks to the desired termination tolerance ε_r.

In contrast the RQA shows a superior convergence rate in this simulation. Although the movement in the price-space seems to be chaotic, the collected information helps to identify the equilibrium price after less than 40 iterations. A possible explanation for the large number of iterations that is still needed by both presented methods can be found in the problem structure. While in the unconstrained and quadratic production case in the first case study the shared resources can be adjusted independently from each other, in the case study of INEOS in Köln there seems to be an interdependency of the shared resources that is hidden to the coordinator. In other terms the bounds prohibit an independent increase of one shared resource only.

Analysis of the Response Surfaces

A deeper insight and understanding of the problem structure can be gained by plotting the response surfaces of the network residual for both case studies as shown in Fig. 11. On the horizontal and vertical axes the two prices for the two shared resources are plotted as coordinates. The heat plot shows the constraint violation. For the case study of locally unconstrained plants a strictly quadratic mapping can be identified as in (3.19). In case of the locally constrained case study the situation is different. Although some regions can be described by a quadratic mapping, the influence of the local constraints of the subsystems become visible. The nature of the industrial case study, even with linear economic relations, leads to the situation in which the overall site optimum is governed by the local bounds of the subsystems, which is a well known situation. From a price-based coordination point of view this causes difficulties. Near the optimum the response surface is very sensitive to price changes and shows massive violations when the optimal price is perturbed by just a small value. This can cause instability of the methods and may lead to diverging behavior.

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Discussion

It can be shown that under certain assumptions on the structure of the subproblems price-based coordination is well suited to distribute shared resources among different competing plants. The methodology preserves a maximum of confidentiality by only influencing the subsystems by adjusting transfer prices based on the network balance.

The presented novel price update by recursive quadratic approximation shows a superior convergence rate in the simulation studies and offers potential benefit when it comes to practical implementations, where fewer iterations are key to the success of this strategy. However, it has to be noticed that locally constrained subsystems can pose certain challenges, if the overall site optimum is governed by local bounds. In this case the network balance is very sensitive to price changes and coordination has to be performed with care. Another issue that could be discovered is the interdependency of the shared resources, coupled with inflexible plants, which poses a challenging allocation problem. For the quadratic approximation sophisticated methods for the choice of a reasonable regression set can be applied as shown in [59].

3.2 Price-based Coordination using the Alternating Direction Method of Multipliers

In contrast to the previous section, equations (2.1) can also be solved using methods, whose motivation is rather stability and robustness than speed. Here, stability is defined as guaranteed convergence rate and robustness allows a larger set of mathematical properties for the underlying functions, i.e. not strictly convex ones, as well as for the respective domains in equations (2.1).

3.2.1 Problem Description and Coordination Principle

In the following, these methods are investigated for their application in Model Predictive Control (MPC). Using plant dynamics, transient behavior is taken into account and optimizied, which is the major difference compared to the steady state optimization in Subsection 3.1. In Section 3.2.3, a linear formulation of MPC was introduced. In all N_p intervals, the resource balances have to be fulfilled, which is the motivation for selecting the following methods based on superior convergence properties.

Recently there has been much interest in the application of the Alternating Direction Method of Multipliers (ADMM) and the Inexact Uzawa Method (IUM) on distributed problems of the form (2.1), due to the fact that the convergence of the algorithms can be proved under mild assumptions[26, 60, 39]. In the following, both, ADMM and IUM, are explained for the distributed solution of coordination problems.

Alternating Direction Method of Multipliers

A simple example for a problem that can be solved using sharing ADMM is the problem given in Section 2.1 as (2.1), where we only consider equations (2.1a) and (2.1b).

If we form the augmented Lagrangian, where we enforce the satisfaction of the constraints additionally using a quadratic penalty, we get the following for this problem:

$$\mathcal{L}(U,\lambda) := \sum_{i=1}^{n} J_i(u_i) + \lambda^T \left(\sum_{i=1}^{n} G_i u_i - g \right) + \frac{\rho}{2} \left\| \sum_{i=1}^{n} G_i u_i - g \right\|_2^2 . \tag{3.31}$$

Since this Lagrangian, equation (3.31), is not separable, new variables are introduced and the problem is rewritten

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as

$$\begin{aligned} \min_{U} & \sum_{i=1}^{n} J_i(u_i) \\ \text{s.t.} \;\; & G_i u_i = z_i, \\ & \sum_{i=1}^{n} z_i = g, \end{aligned} \tag{3.32}$$

where the resulting augmented Lagrangian,

$$\mathcal{L}(U, \lambda) := \sum_{i=1}^{n} J_i(u_i) + \lambda^T (G_i u_i - z_i) + \frac{\rho}{2} \|G_i u_i - z_i\|_2^2 + \mu^T \left(\sum_{i=1}^{n} z_i - g \right), \tag{3.33}$$

is now separable in decision variables u_i. The variables z_i can be interpreted as vectors of proposed shared resource utilization for system i, with $\dim(z_i)$ equal to the number of shared resources and n the number of subsystems. The price vector $\lambda \in \mathbb{R}_+^g$ and the penalty term $\rho \in \mathbb{R}_+$ are the dual variables of the Lagrangian relaxation and the augmented Lagrangian term in the objective.

From the Karush-Kuhn-Tucker conditions we get the iteration scheme with the local minimization of the extended Lagrangian function

$$u_i^{k+1} = \underset{u_i}{\text{argmin}} \; J_i(u_i) + \lambda^{k,T} (G_i u_i - z_i^k) + \frac{\rho}{2} \left\| G_i u_i - z_i^k \right\|_2^2, \tag{3.34}$$

and update rules for μ, z_i and λ:

$$\mu^{k+1} = \lambda^k - \frac{\rho}{n} \left(g - \sum_{i=1}^{n} G_i u_i^{k+1} \right), \tag{3.35}$$

$$z_i^{k+1} = \frac{\lambda^k - \mu^{k+1}}{\rho} + G_i u_i^{k+1}, \tag{3.36}$$

$$\lambda^{k+1} = \lambda^k + \rho \left(\sum_{i=1}^{n} G_i u_i^{k+1} - z_i^{k+1} \right). \tag{3.37}$$

For more details about the ADMM approach, the reader may refer to [39, 4]. It has been shown that the convergence rate of ADMM is $O(\frac{1}{k})$ in the worst case [61]. If the local objective functions are strongly convex, [62] states that linear convergence is guaranteed for the following algorithm. The solution algorithm is presented (Algorithm 1).

Inexact Uzawa Method

The inexact Uzawa method [63] is an even more conservative modification of the ADMM, which employs an additional augmented Lagrangian term. The difference between IUM and ADMM is the re-formulation of the distributed optimization problems as in (3.38), where the additional term penalizes the changes of the variable u_i between the iterations.

$$u_i^{k+1} = \underset{u_i}{\text{argmin}} \; J_i(u_i) + \lambda^{k,T} \left(G_i u_i - z_i^k \right) + \frac{\rho}{2} \left\| G_i u_i - z_i^k \right\|_2^2 + \frac{1}{2} \left\| u - u^k \right\|_D^2, \tag{3.38}$$

where D is a block-diagonal weighting matrix. If $D = 0$, the inexact Uzawa method is identical to ADMM, however for any $D \succ 0$ the sub-problems are strictly convex which generally is not the case of ADMM. Note that apart from this, IUM inherits the general convergence properties of ADMM.

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Data: ρ, λ^0, k_{max}, ϵ, δ, n
$z_i^0 := 0$, $k := 0$;
Result: λ^*, u_i^*, z_i^*
while $k < k_{max}$ **do**
  for $i = 1 : n$ **do**
    $u_i^{k+1} := \text{argmin}_{u_i} \mathcal{L}_i \left(u_i, z_i^k, \lambda^k\right)$;
  end
  if $\left(\|\sum_{i=1}^n G_i u_i - g\|_\infty < \epsilon \text{ and } \Delta u^k \leq \delta\right)$ **then**
    $\lambda^* := \lambda^k$, break;
  else
    $\mu^{k+1} := \lambda^k - \frac{\rho}{n}\left(g - \sum_{i=1}^n G_i u_i^{k+1}\right)$;
    $z_i^{k+1} := \frac{\lambda^k - \mu^{k+1}}{\rho} + G_i u_i^{k+1}$;
    $\lambda^{k+1} := \lambda^k + \rho\left(\sum_{i=1}^n G_i u_i^{k+1} - z_i^{k+1}\right)$;
  end
  $k = k + 1$;
end

Algorithm 1: Algorithm for price-based coordination using ADMM.

3.2.2 Problem Formulation

To obtain a general problem formulation that can be applied to chemical plants, equation 3.32 has to be rewritten. Reformulating the problem (2.1) into problem (3.39) results in:

$$\min_{u_i} \sum_{i=1}^n J_i(u_i) = \min_{u_i} \sum_{i=1}^n w_i^T u_i = \min_{u_i} \sum_{i=1}^n \left(-p_i^T y_i + p_{ri}^T u_i + p_t^T c_i(x_i, u_i)\right)$$

s.t.

$$\begin{aligned} & F_i(\dot{x_i}, x_i, u_i) = 0, \quad i = 1, \ldots, n \\ & y_i = h_i(x_i), \quad i = 1, \ldots, n \\ & lb_i \leq y_i \leq ub_i \quad i = 1, \ldots, n \\ \\ & R_i(x_i, u_i) = z_i, \quad i = 1, \ldots, n \\ & \sum_{i=1}^n z_i = 0. \end{aligned} \tag{3.39}$$

The linear economic objective accounts for the revenue generated by the production, for the raw material cost, and cost for using the infrastructure, which is given by the function c_i. All plant dynamics are contained in the general formulation F_i and the amount of product is determined by h_i. Since production is limited by the demand from the market, each plant has constraints on the amount of product are given by lb_i and ub_i. Hence that, despite the linear (non-strictly convex) objective function and possibly nonlinear dynamics F_i, the decomposition of this problem using ADMM results in the formulation which can be made strictly convex by an appropriate adjustment of the parameter ρ. The price-based coordination formulated this way is then guaranteed to converge to price equilibrium.

3.2.3 Demonstration Example

In order to illustrate the applicability of the price-based coordination scheme we use the case study from the integrated petrochemical site of INEOS in Köln. For this example, the selected case study comprises three plants that are interconnected by resource networks $R_i \in \mathbb{R}^3$ of steam on 5 and 30 bar, and hydrogen. Positive values in R_i denote

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consumption and negative values denote production of the respective shared resource. In the example we consider four products: ethylene (*C2*) and propylene (*C3*) produced by the cracker and ammonia (*Am*) and ammonia water (*AW*) produced in the ammonia plant. The main task of the power plant is to burn the fuel gas from the cracker and to produce the minimum electrical power required for a safety shut-down of the site. The manipulated variables of the power plant are the fuel consumption and the power plant performance factor, which changes the ratio of 5 and 30 bar steam, and thus the electrical power produced. The cracker operation can be set by the naphtha feed and the severity, and the ammonia plant operation depends on the natural gas input. All units decide on their utilization of the shared resources based on the prices set by the coordinator. A simple illustration of the case study is presented in Fig. 1.

Power Plant

We represent the power plant by the following simplified nonlinear model (3.40).

$$\begin{aligned} x_1(k+1) &= A_1 x_1(k) + B_1 u_{11}(k), \\ R_1(k+1) &= S_{A1} x_1(k+1)[u_1(k), 1-u_1(k)]^T, \\ y_1(k+1) &= C_1 x_1(k+1)[u_1(k), 1-u_1(k)]^T, \end{aligned} \tag{3.40}$$

where u_{11} is the fuel gas input and u_{12} the performance factor. The power plant produces electrical power y_1, 5 and 30 bar steam R_1 and it is not connected to the hydrogen network. A_1, B_1 and C_1 represent the system dynamics; S_{A1} and S_{B1} connect the states and the input of the power plant to the shared resources.

Cracker

The cracker is represented in a simplified manner using the following model:

$$\begin{aligned} x_2(k+1) &= A_2 x_2(k) + B_2 u_2(k), \\ R_2(k+1) &= S_{A2} x_2(k+1) + S_{B2} u_2(k), \\ y_2(k+1) &= C_2 x_2(k+1), \end{aligned} \tag{3.41}$$

where u_2 is the input vector of the cracker, the manipulated variables are the naphtha feed, the severity and the 30 bar steam. We consider two output variables of the cracker y_2 - ethylene and propylene. A_2, B_2 and C_2 represent the system dynamics, S_{A2}, S_{B2} are the matrices that map the state and the inputs to the shared resource utilization R_2. The cracker produces hydrogen and consumes 5 and 30 bar steam.

Ammonia Plant

The ammonia plant processes natural gas and hydrogen (u_3) to produce ammonia and ammonia water (y_3). A_3, B_3 and C_3 represent the system dynamics and S_{A3}, S_{B3} are the matrices that map the state and inputs to the shared resource utilization R_3. The ammonia plant produces 30 bar steam and consumes hydrogen and 5 bar steam.

$$\begin{aligned} x_3(k+1) &= A_3 x_3(k) + B_3 u_3(k), \\ R_3(k+1) &= S_{A3} x_3(k+1) + S_{B3} u_3(k), \\ y_3(k+1) &= C_3 x_3(k+1), \end{aligned} \tag{3.42}$$

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3.2.4 Implementation and Results

We formulate the local optimization problem for plant i as an economic optimization problem with a look-ahead horizon of $N_p = 3$ hours and a sampling time of 15 minutes. The local problem can be be formulated as follows:

$$\begin{aligned} \min_{u_i} \; & (-p_i^T y_i + p_r^T u_i + p_t^T c_i(x_i, u_i) + \lambda^T (R_i(x_i, u_i) - z_i) + \frac{\nu}{2} \|R_i(x_i, u_i) - z_i\|_2^2) \\ \text{s.t. } & F_i(\dot{x_i}, x_i, u_i) = 0, \\ & y_i = h_i(x_i), \\ & lb_i \leq y_i \leq ub_i \end{aligned} \tag{3.43}$$

where the variables have dimensions adopted to the length of the prediction horizon, i.e. $u_i \in \mathbb{R}^{m_i \times N_p}$, $y_i \in \mathbb{R}^{N_y \times N_p}$, where N_y is the number of output variables. The coordinator initializes and updates the prices of the shared resources λ for all units. After performing the local optimization, each unit replies with a vector of the utilization of the shared resources R_i^k in iteration k. Then the error in each of the shared resource networks is calculated as $E(k) = \sum_{i=1}^{n} R_i^k$ and if the global constraints are not satisfied, the primal variables and the price of the shared resources are updated. The iterations are performed at any sampling time and the converged variables are then applied until the end of the next sampling interval. So the local optimizers may be queried many times at each sampling time. To quantify the convergence of the coordination approaches we use the primal infeasibility of the coupling constraint (3.44).

$$\frac{\| \sum_{i=1}^{n} R_i^k \|_\infty}{\max\left(1, \| \sum_{i=1}^{n} R_i^0 \|_\infty\right)} \leq \epsilon. \tag{3.44}$$

The local controllers and the coordinator are implemented in MATLAB and are connected to the modeling, simulation and validation framework developed in DYMASOS as black-box components after compilation as shared libraries using the MATLAB compiler and via the DLL interface. The implementation details are the same as the information given in Section 3.1.5. The local controllers iterate with the coordinator via a Modelica-based event interface which is explained in detail in D4.1. For more details on the event iteration concept in Modelica, the reader is referred to [64].

Both ADMM and IUM were tested for different scenarios. The results shown here were obtained considering by gradual changes of the demand of ethylene, propylene and ammonia as shown in Fig. 12. The total simulation time is 85 hours, $\nu = 0.5$ and the price vector was initialized as $\lambda = [12, 12, 15]^T$. For the IUM the penalty function for the deviation of the previous iteration is $D = \mathbf{I} \cdot 10^{-2}$. The results are compared to a centralized optimization where we assume that all information regarding the internal structure and constraints of the subsystems is available. The optimal values for the manipulated variables and production rates obtained from the centralized solution are denoted by u^* and y^*.

The primal infeasibility (3.44) of the solution by ADMM and IUM versus the iteration number in time $t = 0$ is depicted in Fig. 13. We can notice that if properly tuned, both algorithms have satisfactory convergence properties.

Figure 14 presents the results for the deviations of the production levels from the centralized solution y^* for both algorithms is presented. The results for ADMM are marked with solid red line and IUM with dashed blue line. We can note that the coordination algorithms successfully drive the system towards the plant-wide optimum. In each interval, the deviations of the manipulated variables from the centralized solution u^* are close to 0, see Fig. 15.

The main drawback of the algorithms for price-based coordination is the number of iterations needed to calculate the equilibrium price. The necessary number of iterations is strongly dependent on the tolerance, and for tight tolerances may rapidly increase. In our case the large system of pipes that is interconnecting the different units in the integrated petrochemical site can serve as a buffer for balancing small errors, so a high precision of the coordination algorithm is not needed and the algorithm can be terminated for a constraint violation of $\delta = 0.05$. The number of iterations needed to achieve this tolerance is shown in Fig. 16 and the calculated equilibrium prices for the shared resources are depicted in Fig. 17. Obviously during steady state operation, the equilibrium prices have constant values, but whenever there is a change in the demands of the products, fast dynamic changes in the equilibrium price value can be observed. Figure 17 also shows that the optimization may terminate at slightly different prices if the tolerance is not very small.

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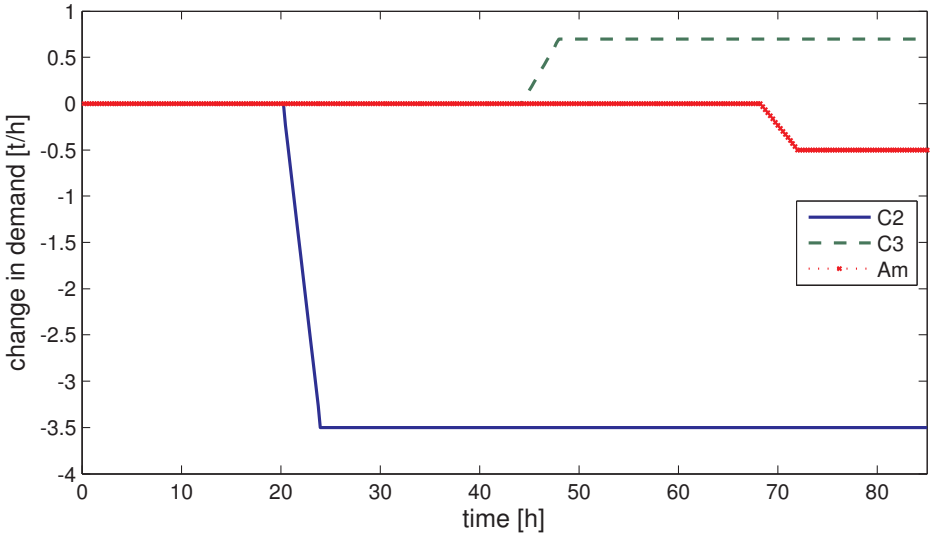

Figure 12: The change in demand of ethylene, propylene and ammonia.

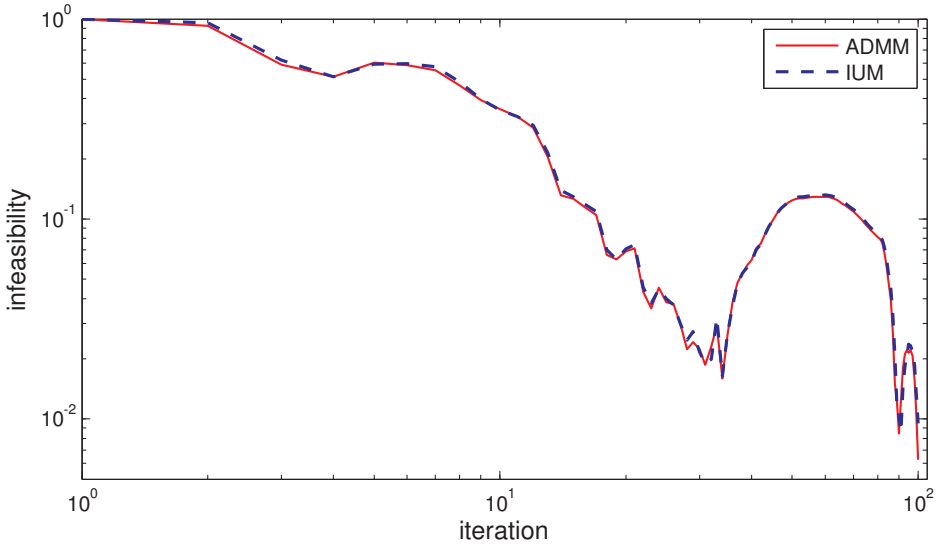

Figure 13: The primal infeasibility versus the iteration number for time t=0.

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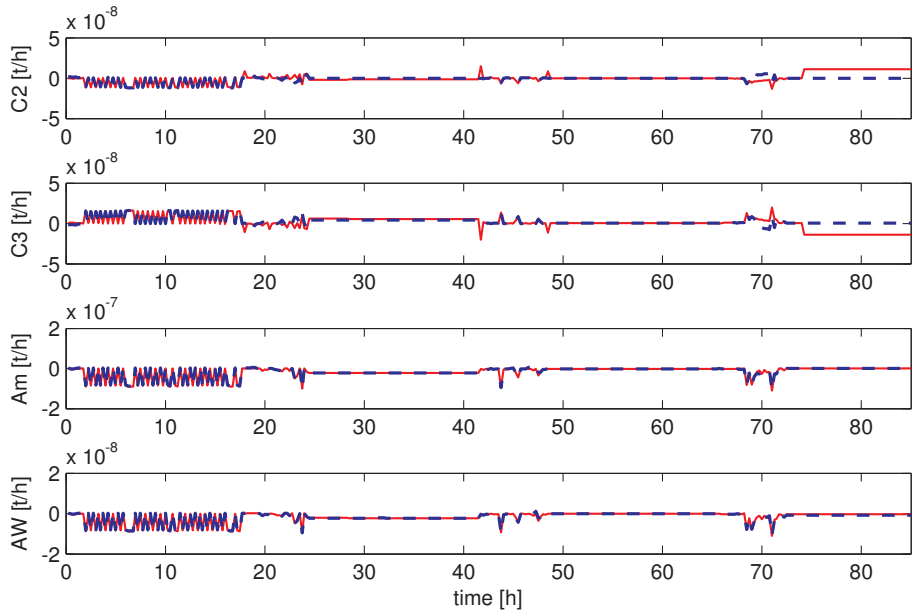

Figure 14: Deviation of production from the centralized solution $y^* - y_i$ (ADMM-solid red; IUM-dashed blue).

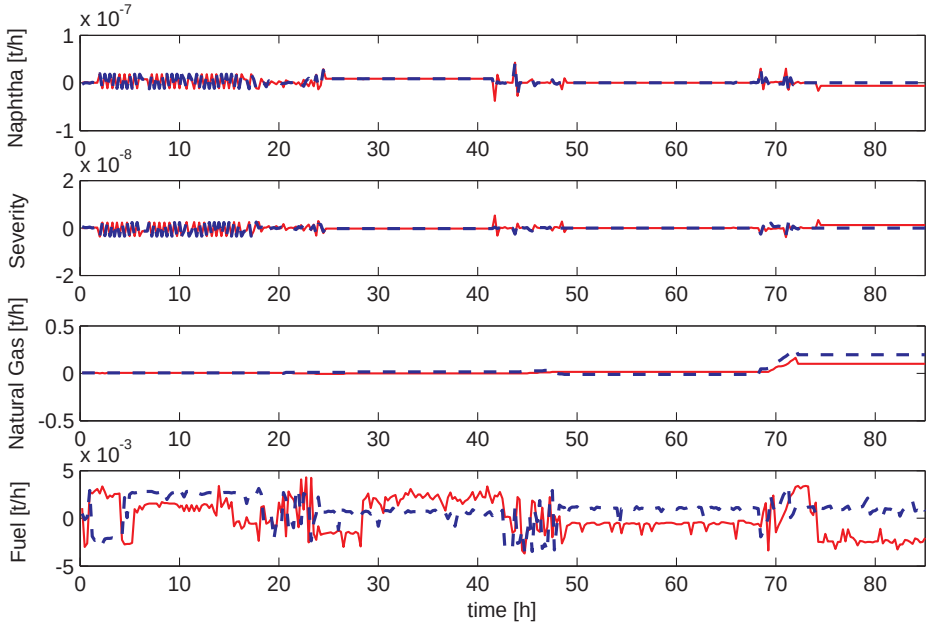

Figure 15: Deviation of manipulated variables from the centralized solution $u^* - u_i$ (ADMM-solid red; IUM-dashed blue).

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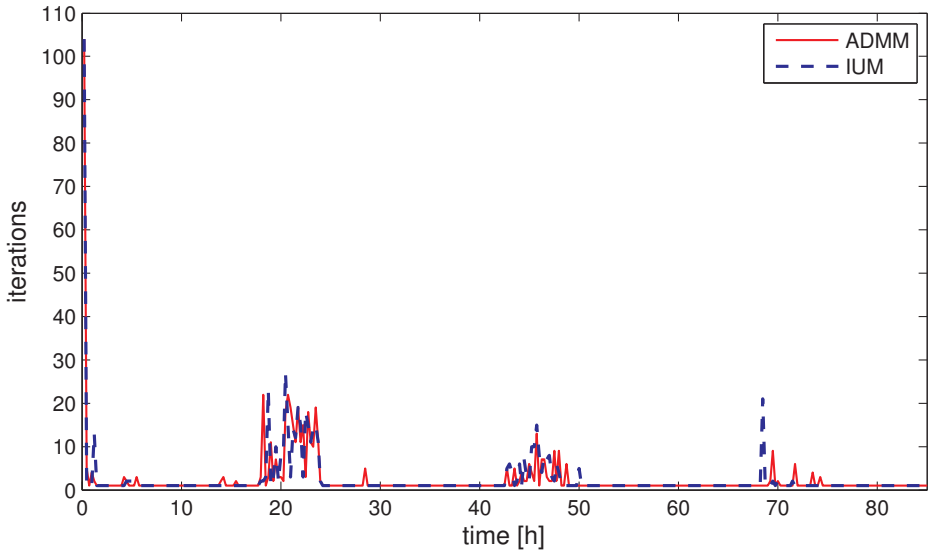

Figure 16: Number of iterations of the coordination method in each step.

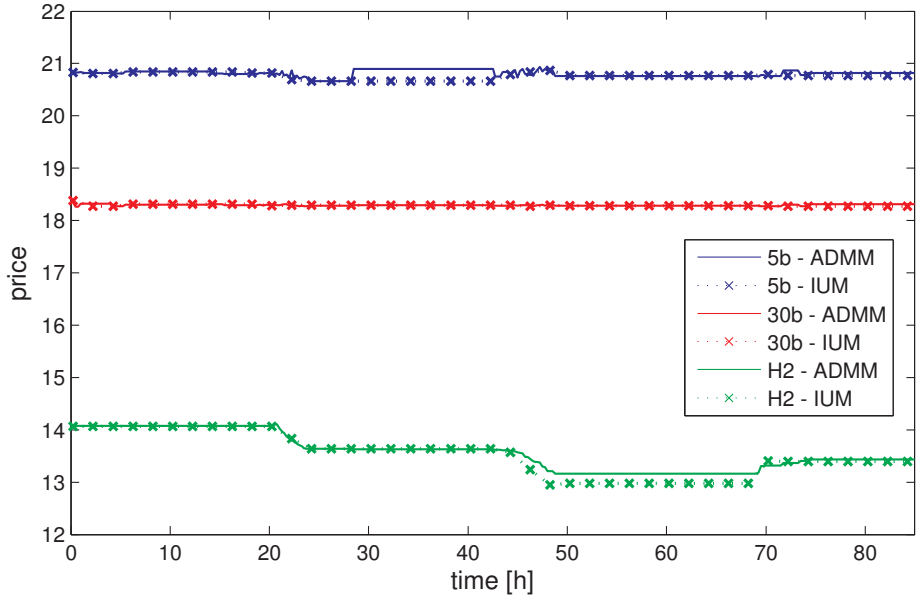

Figure 17: Equilibrium price.

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4. Extension of Market-based Coordination to Coordination of Coupled Batch Production Units

This formulation is now extended for discontinuous production processes, where the prediction horizon is not fixed in time but a function of the inputs.

4.1 Problem Description and Coordination Principle

Especially in the process industry, both for chemical and, even more so, biological processes, many production processes are carried out in batch or semi-batch mode. This results mainly from two reasons, the possibility to switch between different products and the high flexibility in terms of temperature control. To overcome the disadvantage of limited reactor capacity, that results from various reasons e.g. geometric properties, and to still produce the necessary volumes of various products, it is common to operate several batch reactors as one plant, where upstream and downstream units as well as resources, such as equipment or utilities and raw materials, are shared.

Even though up- and downstream parts are continuous processes, the inherent discontinuous operation of batch and semi-batch processes requires different steps to be taken. In the following, the operation of chemical reactions in semi-batch mode is used as example. Most commonly, these are the following ones:

- Inerting: Setting up the correct atmosphere inside the reactor
- Filling: Preparing the reaction phase by adding for example catalyst and starter
- Reaction: Feeding the critical component
- Post-reaction: Finishing and cooling of the product
- Emptying: Discharge of the product to subsequent units
- Cleaning: Preparing the reactor for the next operation

In the general case and assuming that all discontinuous resources are appropriately scheduled, all steps except from reaction and post-reaction have a fixed duration, which is why those two and especially the reaction phase can be tweaked using dynamic optimization. If the batch time can be decreased, with it, the net time of the whole production can be reduced and thence profitability increased. Hence the minimization of the reaction phase has increasingly entered industrial environments [65, 66, 67]. As already proposed in [68], in the following the minimum batch time problem for several semi-batch reactors sharing resources is considered. Along with a centralized plant wide minimum time optimization problem, local optimization of the individual reactors coordinated by an overarching iteration scheme is investigated for the following reasons: Larger robustness, easier industrial implementation, and higher transparency for plant operators.

4.1.1 Optimal Sequence Evaluation

Dynamic optimization has been done primarily for single reactors, such as in the work by e.g. by [67] and [69]. Simultaneous operation of several reactors have been investigated in the context of scheduling the necessary steps for optimal operation. A good summary is given, for example, in [70]. However, only limited reactor dynamics are accounted for in the optimization, which is why it gives good feasible solutions, but still allows for improvement. Thence, combined scheduling and control has become a intensively researched topic in the past years [71].

Here, a minimization of the overall batch time of several, parallel running batch plants that share resources is done, by simultaneously optimizing overall plants at once. A common objective for the minimization of batch times is to

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$\sum$	$u_{1,1}$	$u_{2,2}$	$\dots$	$u_{nReac,nInt-1}$	$\leq$	u_{max}
$\sum$	$u_{1,2}$	$u_{2,3}$	$\dots$	$u_{nReac,nInt}$	$\leq$	u_{max}
$\vdots$	$\vdots$	$\vdots$	$\dots$	$\vdots$	$\vdots$	$\vdots$
$\sum$	$u_{1,nInt}$	$u_{2,1}$	$\dots$	$u_{nReac,nInt-2}$	$\leq$	u_{max}

Table 2: Cyclic formulation of the constraints on all reactors (columns) for the shared resources for every discretization interval (rows)

find the optimal trajectory by maximizing the feed flow rates. This however, is only possible, if all resources, except from the feed flow rate, are available at a constant predefined level for each plant. Here, the assumption is that the plants share more than one limited resource, e.g. flow rates of coolant and feed streams, and thence a simple transformation of the objective is not possible. Instead, a dynamic distribution of the shared resources must be taken into account and the objective is indeed to minimize the time t_{Final}.

When considering several reactors of the same type, there are different ways to express the minimum batch time. If several reactors start at the same time, the last to finish determines the final batch time. Otherwise, the objective of the optimization can be either formulated as the sum of the individual reaction times, the time between the starting of the first and finishing of the last reactor, or a combination of both. In general, the first case will result in as little overlap of the reaction phases as possible and the second formulation will result in a short batch time for the one that started last and longer ones for the remaining reactors. Therefore, a combination of both formulations is used here. The sum of all individual batch times is minimized with the additional constraint that the batch times have to be equal for all reactors.

In general, the goal is not to optimize a single sequence of a given number of batches, but to find the optimal operation of a continuing sequence of batches. So we assume that after a batch is finished, the next batch will be started, neglecting the intermediary steps, since they are of fixed durations. Cyclic constraint formulations, as shown in Table 2, can be used to express the proposed problem formulation. The constraints on the shared resources have to be satisfied in every time interval. In Table 2, the operation of reactor $i = 2$ is exemplary shifted by one and reactor $i = nReac$ by $nInt-2$ intervals. The starting times of the different reactors can written as a tuple $(1, 2, \dots, nInt-1)$.

4.1.2 ADMM Consensus and Inequality Constraint Sharing

In the following, dual decomposition, for shared resource allocation problems, and the alternating direction method of multipliers (ADMM), for solving the consensus problems, are used, which are explained in this section.

In general, a minimization problem with a strictly convex objective function of the form $J^{share}(u) = \sum_{i=1}^{n} J_i^{share}(u_i)$, with $u_i \in \mathbb{R}_i^m$, $JG^{share} : \mathbb{R}_1^m \times \mathbb{R}_2^m \times \dots \times \mathbb{R}_n^m \to \mathbb{R}$, and $n \geq m$, is called separable, since the function J^{share} is composed of n individual functions J_i^{share}, e.g. representing the objective functions of the subsystems. If this problem is subject to global constraints $\sum_{i=1}^{n} G_i^{share} u_i = g$, for instance the necessity to balance resource networks, the global constraints can be relaxed by adding them to the objective function and formulating the Lagrangian:

$$\mathcal{L}(U, \lambda) = \sum_{i=1}^{n} \mathcal{L}_i(u_i, \lambda) = \sum_{i=1}^{n} \left(J_i^{share}(u_i) + \lambda^T G_i^{share} u_i - \frac{\lambda^T}{n} g \right). \tag{4.1}$$

The constraint is multiplied by $\lambda \in \mathbb{R}_+^g$, which at the optimum can be interpreted as the cost associated with the relaxation of the constraint. In Equation (4.1) can be seen that the Lagrangian is also separable.

The minimization problem of $J_1(U)$ can be solved by iterating between minimization of the N Lagrangians with respect to u_i, the so called primal problem, and the dual problem, where the Lagrangian is maximized with respect to λ and primal feasibility, i.e. satisfaction of the constraints is achieved, by using, for example, a subgradient method. If the coupling between different systems is present within the objective, such as $J^{cons}(U) = \sum_{i=1}^{n} J_i^{cons}(u)$, where different subsystems want to achieve a certain common goal, the problem can be transformed into a separable problem by transforming the common variable, u, to local ones, u_i, and adding the "copy constraints" $u_i = z$ to the

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respective objective functions. However, additionally to the steps from the previous solution method, an update of the variable z is required in each iteration, which is then called ADMM.

If the problem is very sensitive to changes in the common variable u and to speed up convergence, an augmented Lagrangian can be used, where the 2-norm of the constraint multiplied by a penalty factor $\frac{\rho}{2}$ is added to the objective [4]. These two types of problems, the minimization of J^{cons} and JG^{share} are called sharing and consensus problems, respectively, and dual decomposition can be applied to solve both types of optimization problems.

We consider a problem that has the characteristics of both problems

$$\begin{aligned} &\min_{U} \sum_{i=1}^{n} J_i(u_i) \\ &\text{s.t.} \sum_{i=1}^{n} \begin{pmatrix} G_i^{share} \\ G_i^{cons} \end{pmatrix} u_i = \begin{pmatrix} g \\ 0 \end{pmatrix}, \end{aligned} \tag{4.2}$$

where the matrices G_i^{share} and G_i^{cons} are formulated according to equation (2.2) and (2.4) respectively. Then the Lagrangian can be formulated as

$$\mathcal{L}(u, \lambda_{cons}, \lambda_{share}) = \sum_{i=1}^{n} \left(J_i(u_i) + \lambda_{cons,i}^T (u_i - z) + \frac{\rho}{2} \|u_i - z\|_2^2 + \lambda_{share}^T G_i^{share} u_i - \frac{\lambda_{share}}{n} g \right).$$

Optimization via dual decomposition of Problem (4.2) is done by iteratively dual problem equation (4.3). The resulting iteration scheme to find the optimum is the following, where the constant term is neglected in the local minimization:

$$u_i^{k+1} = \arg\min_{u_i} \left(J_i(u_i) + \lambda_{cons,i}^{T,k} (u_i - z^k) + \frac{\rho}{2} \left\| u_i - z^k \right\|_2^2 + \lambda_{share}^{T,k} G_i^{share} u_i \right), \tag{4.3}$$

$$z^{k+1} = \frac{1}{n} \sum_{i=1}^{n} \left(u_i^{k+1} + \frac{\lambda_{cons,i}^k}{\rho} \right), \tag{4.4}$$

$$\lambda_{cons,i}^{k+1} = \lambda_{cons,i}^k + \rho \left(u_i^{k+1} - z^{k+1} \right), \tag{4.5}$$

$$\lambda_{share}^{k+1} = \lambda_{share}^k + \alpha \left(\sum_{i=1}^{M} G_i^{share} u_i^{k+1} - g \right). \tag{4.6}$$

Equation (4.3) is the minimization of the Lagrangian, which can be done in parallel due to the separable problem structure. Equations (4.4) and (4.5) update the global copy z of the local variables u_i and the Lagrange multipliers $\lambda_{cons,i}$ to improve consensus. Equation (4.6) updates the sharing Lagrange multipliers, λ_{share}, in order to improve the satisfaction of the sharing constraints. Due to the dual decomposition, each subsystem can solve a local optimization problem without communicating its local objective function J_i or underlying model equations. Information about the overall problem is communicated from the coordinator to the subsystems via the "prices" λ_{share} and $\lambda_{cons,i}$.

4.2 Problem Formulation

The input domain is discretized using direct multiple shooting to transform the continuous problem into a discrete one where the cyclic constraints are imposed on each shooting interval.

$$\begin{aligned} \underset{u_{i,j}}{\text{minimize}} \quad & \sum_{i=1}^{nReac} t_{f,i} \\ \text{subject to} \quad & F_i(u_{i,1}, \ldots, u_{i,nInt}, t_{f,i}) = 0, \qquad \forall i = 1, \ldots, nReac, \\ & t_{f,1} = t_{f,2} = \cdots = t_{f,nReac}, \\ & \sum_{i=1}^{nReac} u_{i,j=\text{shift(i)}} \leq u_{max} \quad \forall j = 1, \ldots, nInt, \qquad \text{see Table 2.} \end{aligned} \tag{4.7}$$

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The minimum batch time optimization for batch reactors with shared resources is formulated as Problem (4.7), where $F_i(u_{i,1}, \ldots, u_{i,nInt}, t_{f,i}) = 0$ contains dynamics and local constraints. The $j = \text{shift(i)}$ operator, adjusts the index j of reactor i according to the starting value from the triple.

4.3 Demonstration Example

To demonstrate this approach, isothermal semi-batch reactors with safety constraints from [65] are considered. In a second order reaction, reactant A and B react to product C. The mass balance is given by the differential equations (4.8), (4.9), and (4.10).

$$\frac{\mathrm{d}c_A}{\mathrm{d}t} = -kc_Ac_B - \frac{u}{V}c_A, \tag{4.8}$$

$$\frac{\mathrm{d}c_B}{\mathrm{d}t} = -kc_Ac_B - \frac{u}{V}\left(c_{Bin} - c_B\right), \tag{4.9}$$

$$\frac{\mathrm{d}V}{\mathrm{d}t} = u, \tag{4.10}$$

$$c_C = \frac{c_{A0}V_0 + c_{C0}V_0 - c_AV}{V}, \tag{4.11}$$

$$T_{cf}(t) = T(t) + \min(c_A(t), c_B(t))\frac{-\Delta H_R}{\rho c_p}. \tag{4.12}$$

The algebraic equation (4.11) results from the product concentration depending on the differential states. The problem is interesting due the presence of three different types of constraints:

- Path constraints: The reactors are operated isothermally, however for safety reasons the event of a cooling failure is considered and the peak temperatures at cooling failure, $T_{cf,i}$, given by equation (4.12), must always be below T_{max}.
- Terminal constraints: The final time of the reactions are defined by the desired amount of C in the reactors and the volume in the reactors must not exceed a maximum capacity, $V_{max,i}$.
- Input constraints: The feed rates $u_{i,j} \forall j$ of reactant B are constrained to be less than $u_{max,j}$.

Additionally to the local constraints, the overall sum of all feed flow rates (see Table 2) of reactant B must be less or equal to $u_{max} = 0.04\,\mathrm{l/h}$ within each interval. The initial concentration of B in the reactors and the initial volume are assumed to be $c_{B,0} = 0.55\,\mathrm{mol/l}$ and $V_0 = 0.6\,\mathrm{l}$ such that the individual optimal input profiles consist of three different arcs. The remaining parameters are taken from Table 3 in [65]. The case study is evaluated for three reactors and five shooting intervals. The parameters z, $\lambda_{cons,i}$, and λ_{share} are initialized with zero and the tuning parameters α and ρ are empirically chosen to be 25 and 0.1.

4.4 Implementation and Results

Since the three reactors are equal, the number of different reactor configurations (triplets) that have to be investigated can be reduced from 125 to 7. These triplets are:

$$(1,1,1), (1,1,2), (1,1,3), (1,1,4), (1,1,5), (1,2,3), (1,2,4).$$

Those configurations of Problem (4.7) are solved by hierarchical coordination and the results are compared with the centralized solution, which are given in Table 31. The local optimization and the central optimization are done using CasADi [72] with IPOPT [73]. For the hierarchical solution, relative primal and dual tolerances are set to be $Tol = 10^{-6}$.

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Triplet	(1,1,1)	(1,1,2)	(1,1,3)	(1,1,4)	(1,1,5)	(1,2,3)	(1,2,4)
t_{Final} [h]	29.488	27.865	26.893	26.723	27.490	26.273	25.707

Table 3: Minimum batch time for three reactors starting at the intervals given by the triplets.

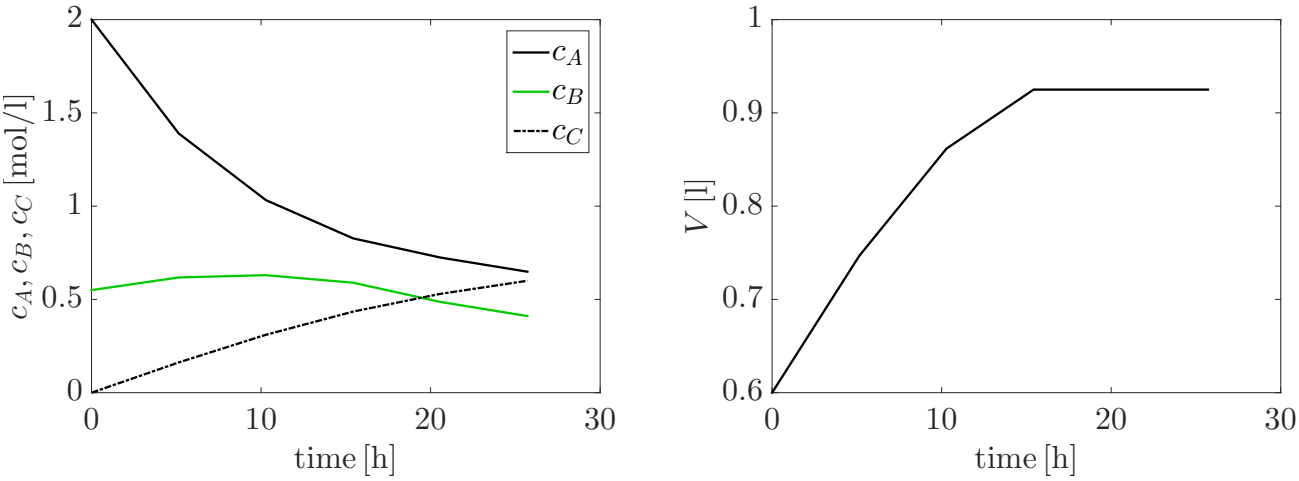

Figure 18: Trajectories of concentrations (left) and liquid volume (right) over the reaction time for reactor one of the starting time triplet (1,2,4).

4.4.1 Analysis of the Centralized Solution

The batch times, calculated with the hierarchical and validated using the centralized scheme, are shown in Table 3. As expected, the shortest batch time can be achieved when the starting points of the reactors are the furthest from each other. While for the trivial case (1,1,1), where the shared resources are distributed evenly, the path constraints are not active, they are active for all other configurations. Exemplary, the concentrations, the liquid level, and the liquid volume of reactor one are shown in Fig. 18 for the starting time triplet (1,2,4). The concentration c_C reaches the terminal constraint of $0.6\,\mathrm{mol/l}$ at the end of the reaction. Furthermore, the path constraint on c_B given by the bound on T_{cf} is active at $0.6\,\mathrm{mol/l}$.

4.4.2 Analysis of the Hierarchical Solution

Figure 19 shows the satisfaction of the global constraints, the development of the prices for shared resources, and the development of the objective functions of the hierarchical optimization.

One can see that the sums of the feed rates switch between being constant and changing very rapidly (see Fig. 19 (top-right)) until they start to converge smoothly towards the constraint. The constant parts are the result of active local constraints that, if inactive, allow rapid changes in the solution structure.

The final time $t_{f,i}$ starts for all reactors at the optimal solution of the local problem without global constraints and then rises until it reaches its final value. Consensus and sharing have to be established at the same time and the influence of t_{Final} is more significant on the remaining global constraints then vice versa. Therefore consensus is enforced using ADMM, which strongly limits the degree of freedom with respect to t_{Final} and allows the systems to converge to global optimality.

Looking at the number of iterations, two distinct phases can be distinguished. The first 400 iterations are used to find the right price structure and the $u_{i,j}$ vary significantly. The remaining iterations are necessary to fine tune the prices in order to fulfill the tolerances. To reduce the number of iterations necessary to find the correct price structure, one could initialize the prices with estimates from previous solutions. The iterations due to the readjustment of the prices, however, are caused by the convergence rate, which is only proven to be $\mathcal{O}(1/k)$, where k is the number of iterations [74]. Nonetheless, there might be methods that are better suited to maximize the dual function without

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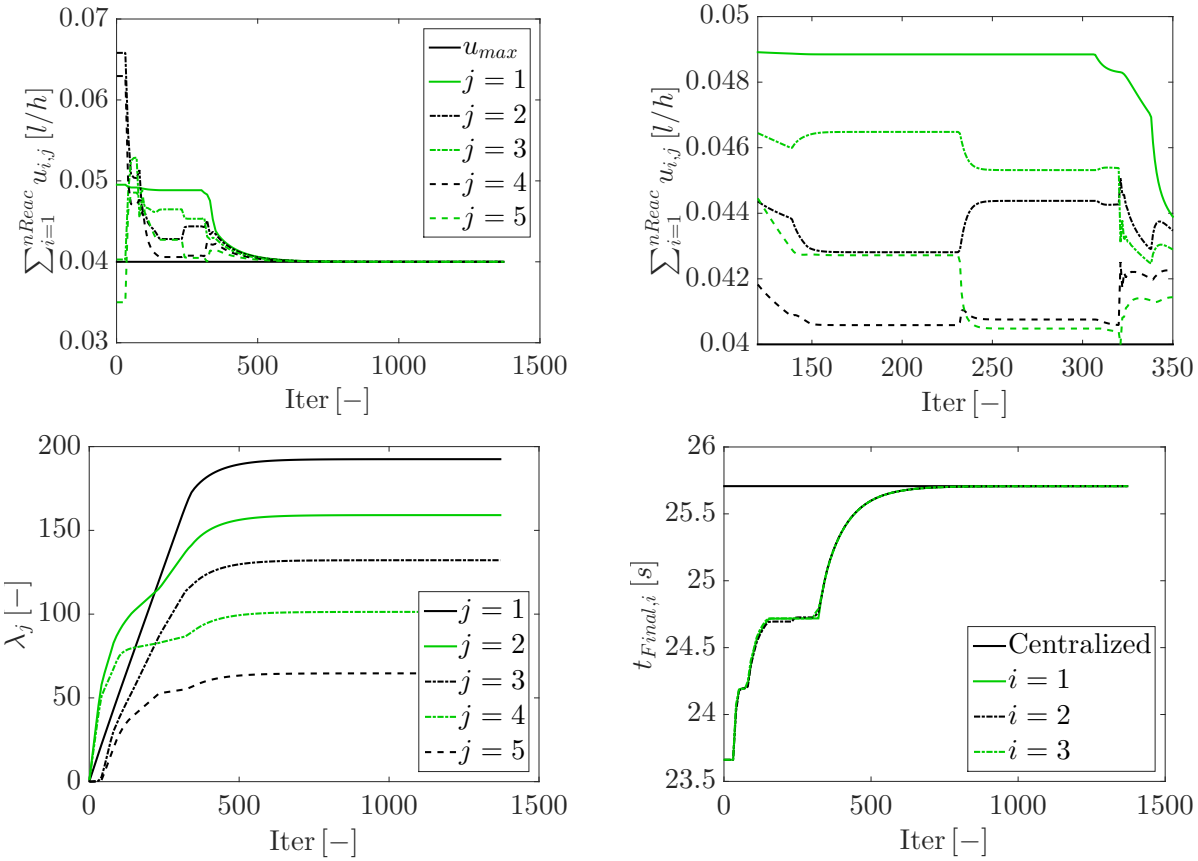

Figure 19: Use of the shared resources (top-left) and magnification to show constant and fast changing profiles (top-right); evolution of the prices for the shared resources (bottom-left) and of the final times of the individual reactors (bottom-right).

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guarantees on convergence rates that depend on the given problem.

4.4.3 Discussion

The hierarchical solution of a distributed minimum batch time optimization with shared resources was discussed. Convergence within predefined tolerances was demonstrated, however the number of iterations needed to converge to the optimal solution is large. The proposed method results in the best sequence of utilization of the shared resources. Future research includes investigations on adaptive tuning of the parameters ρ and α, the use of methods from derivative free optimization to maximize the dual function, and to apply the technique to an industrial semi-batch reactor case.

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5. Conclusions

This document provides a report on market-based coordination strategies developed in the Workpackage 2 of the DYMASOS project. We presented the set of problems, related to the case studies defined in the WP 5 of the project, that arise in processing industries in the context of operational independence of constituting systems, i.e. a characteristic feature of systems of systems. We briefly reviewed the approaches, present in the literature, based on market-like coordination mechanisms that steer the behavior of the constituent systems of a (cooperative) system of systems to fulfill a common goal under present coupling in the form of shared resources. We presented the developments which provide extensions to the state-of-the-art methodologies of price-based coordination. These, on one hand, establish efficient (fast-convergent) price-based coordination and, on the other hand, enlarge the domain of applicability of this type of coordination to problems involving non-strictly convex objective functions of local management problems, stringent local constraints, and discontinuous production units. We also briefly discussed the implementation of the proposed algorithms into the simulation platform that is developed in WP 4 of the DYMASOS project, which allows for seamless transition of the research presented here to action at the real-world engineering problems. Several examples, of varying complexity, were provided to illustrate the basic features of the reported methods and give a concrete outlook of the applications of these methods for the case studies of DYMASOS. The algorithmic developments presented in this report will be further applied to the case studies from the area of chemical industry provided by partners BASF and INEOS for demonstration of their applicability as one of the final results of DYMASOS.

The extensions to the proposed methodological developments in the framework of price-based (market-based) coordination can be summarized:

1. Speed of convergence
   The rate of convergence (especially for ADMM-based algorithms) should be further enhanced. One possible way is to use similar techniques, as presented in the Section 3.1.3, which use features of gradient-free optimization.

2. Problem type
   It should found out how to tune the price-based algorithm using quadratic approximation and ADMM algorithm such that the convergence of the coordination can be guaranteed for the problems that involve piece-wise linear, nonlinear and nonconvex functions.

3. Vertical integration
   The problems presented here look at the problem of horizontal integration, i.e. the constituting systems of SoS belong to one decision layer where they interact tightly with each other, e.g. they share the resources. It should investigated whether the presented coordination principles could be applied to the problem where two or more layers of the decision pyramid (e.g. RTO and MPC layers or scheduling and batch optimization layers) are integrated in similar fashion.

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