Available online at www.sciencedirect.com
ScienceDirect
Computers and Chemical Engineering 32 (2008) 463–476
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

Integrated scheduling and dynamic optimization of grade transitions for a continuous polymerization reactor

Adrian Prata [a,1], Jan Oldenburg [b,2], Andreas Kroll [a,3], Wolfgang Marquardt [b,*]

[a] *ABB Corporate Research, D-68526 Ladenburg, Germany*
[b] *Lehrstuhl für Prozesstechnik, RWTH Aachen University, D-52056 Aachen, Germany*

Received 18 December 2005; received in revised form 6 March 2007; accepted 12 March 2007
Available online 23 March 2007

Abstract

This paper presents a modeling and numerical solution method for an integrated grade transition and production scheduling problem for a continuous polymerization reactor. The optimal sequence of production stages and the transitions between them is supposed to be determined for producing a given number of polymer grades at certain amounts and quality specifications in the most economical way. The production schedule has to satisfy due dates for specific orders. This operational problem is cast into a mixed-integer dynamic optimization problem. Disjunctions and logical constraints are combined with a validated differential–algebraic model describing the polymer process during the production of a specific grade as well as along a transition between two different grades. The modeling and solution approach proposed by Oldenburg et al. [Oldenburg, J., Marquardt, W., Heinz D., & Leineweber, D. B. (2003)] is tailored to this problem class to provide an efficient solution technique. An industrial example process serves as an example to illustrate the modeling and solution techniques suggested.

Keywords: Scheduling; Polymer production; Grade transition; Discrete-continuous dynamic optimization; Disjunctive problem formulation; Mixed-logic dynamic optimization

1. Introduction

During the last decades the competition in the process industries has sharply increased due to global and saturating markets. This is particularly true for commodities such as bulk petrochemicals and even some polymers such as polyolefines. Success in the market can only be achieved if the profitability of the manufacturing process is continuously improved. At the same time, flexible operation of the plants is required to meet the varying demands of customers. A manufacturer has to respond quickly to market needs by adjusting load or grade of the produced chemicals to market demand. Such a situation occurs typically in polymer production where polymer producers are forced to manufacture a variety of grades or qualities of the same polymer requested by the market. These grades are typically produced in production campaigns using the same production plant. To achieve the required agility of the process plants, manufacturing strategies have to be reconsidered in particular for multi-product plants.

The sequence of products manufactured in a production campaign and the transition between the various production phases have to be a decided on in an optimal manner. Nowadays, the production schedule is determined either heuristically or by means of relatively simple process models with fixed processing and transitions times which are obtained from accumulated process know-how. Advanced planning and scheduling (APS) systems are employed on one layer of the automation hierarchy to determine an optimal schedule for a production campaign. This schedule is passed to the advanced control layer of the automation hierarchy where the transition management between production phases has to be implemented. Typically, some multi-variable control system is employed to realize the set-point change, which is required to switch the plant from one grade to another. Improved transitions can be established if dynamic optimization (DO) is employed to first plan optimal reference

* Corresponding author. Tel.: +49 241 80 96712; fax: +49 241 80 92326.
E-mail address: marquardt@lpt.rwth-aachen.de (W. Marquardt).
[1] Present address: Bayer Technology Services, D-51368 Leverkusen, Germany.
[2] Present address: BASF Aktiengesellschaft, D-67056 Ludwigshafen, Germany.
[3] Present address: Kassel University, D-34109 Kassel, Germany.

0098-1354/$ – see front matter
doi:10.1016/j.compchemeng.2007.03.009

Nomenclature

A_g due amount for grade
$B_{\text{low}}^{\text{qv}_n}$, $B_{\text{up}}^{\text{qv}_n}$ lower and upper bounds for the quality variable
cv_n control variables
D_g due amount for grade
f non-linear function for model state derivatives
g^{a} function for the algebraic equations
G number of grades
K set representing total number of stages
$\dot{m}$ production rate
$\dot{m}_{\text{raw}}$ raw material feed flow rate
M_{off} off-special delivery amount produced in stage s
M_{raw} amount of raw material consumed in stage s
MI, SSP used quality variables in case studies (melt index, stereospecifity)
p time invariant parameters
P amount of polymer produced in stage s
qv_n quality variables
S number of stages
t time variable
Δt_s duration of a stage
T_{total} total makespan
u process input
U set representing total number of production stages
V set representing total number of transition stages
W_{T}, W_{raw}, W_{off} weights employed for the objective function formulation
x model state
x_0 initial state
$X_{g,s}$ Boolean variable
$X_{g,s}^*$ binary variable
z algebraic states

Greek symbols
τ dimensionless time variable
ϕ objective function

Subscripts
g for grade index
s for stage index

trajectories on the basis of a rigorous process model, which permits the minimization of the off-spec material produced. The resulting reference trajectories can then be tracked in a delta mode by a PID or model-predictive control system to suppress disturbances and to compensate for plant-model mismatch.

The main focus of the work presented in this paper is the integration of the APS and DO tasks to simultaneously determine the sequence of products in a production campaign and the reference trajectories for realizing the transitions between the production phases in order to achieve an economically more attractive operation of the plant. Rigorous process models reflecting the physico-chemical characteristics of the process are supposed to be used for this purpose to result in an optimal manufacturing strategy with favorable economical properties. The integration of APS and DO has as the major advantage, that the mathematical models and assumptions are consistent in such an integrated approach while they are often in conflict in case of a decomposed approach where APS and DO are treated separately. Further, any decomposition of an optimization problem results in some loss of profit which is avoided by the simultaneous approach. In particular, constraint satisfaction can be systematically enforced by the integrated approach while constraint violations are often encountered in a decomposed strategy. The integration of APS and DO can be expected to significantly contribute to an improved economical performance and to a more robust and safe manufacturing process.

These potential advantages, however, cannot easily be realized. This is due to the fact that the resulting integrated optimization problem is of a discrete-continuous nature since decision-making requires not only to decide on the sequence of products to be manufactured but also on the optimal operating points for each product and on the transitions between the manufacturing phases. Hence, a mixed-integer dynamic optimization (MIDO) problem of considerable complexity has to be formulated and solved for this purpose. In case of polymerization processes the complexity of the continuous part of the problem is largely determined by the high degree of nonlinearity, which often even results in steady-state output or input multiplicity. The discrete part of the problem also shows very high complexity for polymerization processes because of the wide palette of products that is produced by means of the same equipment. An appropriate scheduling and grade transition management of the typically large number of different products ordered by different customers has an immense economical potential. An optimal schedule not only allows to increase productivity but also helps to achieve better coordination, on-time delivery and higher flexibility of the plant.

1.1. Previous related work

Production planning and scheduling has been studied for a long time in both operations research as well as in chemical engineering. Emphasis has been majorly on batch processes and to a lesser extent to continuous processes. Two excellent reviews on the subject have recently been published by Floudas and Lin (2004, 2005) and by Mendez, Cerda, and Grossmann (2006). Generally, the scheduling problem refers to the entire plant and has the aim to ensure a proper sequence for manufacturing a certain number of products over a certain time horizon in order to meet customers' requirements, while minimizing production costs and makespan. It also deals with the allocation of different process units within the complete process flowsheet as well as with the allocation of available resources over time in order to perform a collection of tasks. The scheduling layer generates a production schedule that has to be followed by the lower layers in the automation hierarchy.

Scheduling problems have been formulated in a continuous-time or discrete-time setting (Floudas & Lin, 2004). Popular representations include the state-task network (STN) initially introduced by Kondili, Pantelides, and Sargent (1993) and the resource task network (RTN) proposed by Pantelides (1994). In case of STN representations, the scheduling problem is solved after a discretization of the time coordinate into a number of intervals of equal duration whereas the RTN employs a continuous time representation. The RTN process representation has been adopted later by Castro, Barbosa-Póvoa, Matos, and Novais (2004) who proposed an RTN-based continuous-time short-term scheduling formulation for batch and continuous processes. The authors extended the uniform-grid approach with additional sets of timing constraints for a better relaxation of the formulation results. The continuous tasks are treated here similarly to batch tasks and the formulation resulted in a mixed integer linear programming (MILP) problem. The proposed policy of treating a uniform time grid for all resources might lead to difficulties when a larger number of changeovers is taken into account. The short-term scheduling formulation of continuous multiproduct plants has been addressed by Joly and Pinto (2003) using asphalt production as a case study. The scheduling problem was formulated for eight different final products for a total time horizon of 3 days. The authors have formulated the problem in two different ways, as a mixed-integer nonlinear programming (MINLP) problem and as a MILP problem in which time is uniformly discretized. Computational results for solving both mixed integer programming models are evaluated and discussed.

Dynamic process optimization is concerned with the maximization of profit, while ensuring a safe operation of the plant and with meeting quality targets by calculating optimal set-points or trajectories for the controlled and manipulated variables. There has a lot of research been conducted on dynamic optimization of industrial processes. We will only focus on work related to polymerization in our selective overview. The benefits of optimizing the transitions between two grades in continuous operation have been extensively studied during the last years. McAuley and MacGregor (1992) introduced the basic concepts and applied their methodology to grade transitions for a set of three polyethylene products to determine optimal transition policies. The policy is supposed to avoid the production of off-spec material during transitions. Related work has also been done by Van Brempt et al. (2003). These authors presented a case study where grade transitions have been optimized for a polystyrene production plant subject to an economic objective function.

Some work on the integration of dynamic optimization for the generation of reference trajectories in transient operation of continuous processes with other layers of the plant automation hierarchy can be found mostly in case studies which address the integration of economic optimization and process control. An example has been reported by Tosukhowong, Lee, Lee, and Lu (2004). These authors have used a reduced-order linearized mathematical model for simple continuous process and proposed the integration of the real time dynamic optimization (RTO) layer with different unit controllers. Kadam and Marquardt (2004) and Kadam, Srinivasan, Bonvin, and Marquardt, (2007) presented two alternative approaches for integrating economical dynamic optimization and model-based control to improve operation of continuous process. They apply their methodology to an industrial continuous polymerization process. Chatzidoukas, Perkins, Pistikopoulos, and Kiparissides (2003b) and Chatzidoukas, Kiparissides, Perkins, and Pistikopoulos (2003a) study a problem formulation that permits the simultaneous calculation of optimal transitions and the optimal control configuration by employing a MIDO method. Their case study refers to a gas-phase copolymerization fluidized bed reactor.

There has been only little work on the integration of advanced planning and scheduling with dynamic optimization for the generation of economically optimal trajectories in transient operation of continuous processes. This is largely due to the very different solution approaches. Typically, in scheduling a "time-sequence" approach with fixed or free transition times between production phases is employed and a linear model is employed to result in a mixed integer linear programming (MILP) problem. In dynamic optimization, however, a nonlinear dynamic optimization problem is formulated and solved which accounts for the continuous dynamics of the process. Both problems have been typically solved independently from each other using dedicated solvers which largely prevent an integration of both tasks.

If scheduling and dynamic optimization are integrated, a mixed integer dynamic optimization (MIDO) problem is obtained which is challenging to solve numerically for large-scale nonlinear and hence non-convex problems. The first attempt along those lines has been put forward by Tousain (2002) who chose a full discretization approach to solve the MIDO problem. This author studied the integrated scheduling and dynamic optimization of a continuous blending process and of a high-density polyethylene production plant. More recently, Chatzidoukas et al. (2003a, 2003b) studied integrated scheduling and optimal grade transition using MIDO for a gas-phase polyolefine fluidized bed reactor. These authors treat production stages and the transition stages separately. No detail on the mathematical problem formulation has been given. Gallestey, Stohert, Castagnolli, Ferrari-Trecate, and Morari (2003) employ the framework of hybrid model predictive control to solve scheduling problems by means of MIDO after full discretization of all continuous variables. As a simple case study, the switching between two products each with a dedicated silo has been considered. Dynamic predictive scheduling of a wastewater treatment plant has been addressed using mixed-logic dynamic optimization (MLDO) by Busch, Santos, Oldenburg, Cruse, and Marquardt (2005) and Busch, Oldenburg, Santos, Cruse, and Marquardt (2007). An alternative for the integration of scheduling and dynamic optimization has been suggested by Nyström, Franke, Harjunkoski, and Kroll (2005). Their formulation employs a modular approach where both problems are completely decoupled and solved in an iterative manner. Very recently, Flores-Tlacuahuac and Grossmann (2006) presented a formulation, a solution algorithm and a set of simple case studies for the integrated scheduling and dynamic optimization of continuous-stirred tank reactors. The cases consist of simple problems with one to six differential equations. The problem formulation combines an economical cost function with a least-squares term to force the states and the controls in each stage of the multi-stage problem to desired values. These values have to be determined before by some steady-state optimization problem. The decision variables are the control profiles and the sequence of grades produced in a cyclic schedule. The algorithm is based on a full discretization of the optimal control problem to result in a large-scale MINLP which is solved with standard methods. The method does not allow for a direct optimization of the transition times which have to be determined in an iterative manner. The methodology presented in this paper generalizes the work of previous authors and illustrates the potential of this approach to an industrial case study.

1.2. Outline of this paper

In this article we present a rigorous approach to the modeling and solution of integrated scheduling and dynamic optimization problems. The methodology is illustrated by means of an industrial continuous polymerization process. First, the polymerization process used as a case study is described in Section 2. Second, the mathematical formulation of the proposed integrated policy is given in Section 3. In Section 4 we briefly describe the numerical solution method used for the solution of the overall optimization problem. Optimal production schedules are calculated together with optimal grade transitions in Section 5 for a series of realistic scenarios. Section 6 concludes the paper.

2. The polymerization process case study

2.1. Process description

We consider the simplified flowsheet of a polymerization process, which is typically used for the production of homo- and copolymers of olefins (cf. Fig. 1). The process consists of the homo-polymerization reactor followed by a second reactor typically used for adding a comonomer for copolymer production. The reaction section is followed by a sequence of degassing and receiving silos, which may be operated in a parallel manner. This process section is followed by extrusion, blending, conditioning and packaging units. In this work, we only consider the operation of the first reactor and neglect the downstream process units as a first step the treatment of the complete process problem. The product leaving the first polymerization reactor is already the final polymer product, which can be delivered to customers.

Typically, a large number of grades of the same class of polymers is produced in a sequence of continuous production campaigns (McAuley & MacGregor, 1992). The most important quality specifications defining a polymer grade at the reactor outlet are the melt index (MI) and the stereospecificity (SSP). In the sequel, we replace MI and SSP with qv_n, to result in a more general description of these quality variables. Quality specifications refer to lower and upper bounds of qv_n, which have to be satisfied by the products at any time. The production phases are interlaced by grade transitions where the reactor is switched from one operating point to another in order to meet the quality specifications of the grade to be produced in the subsequent production phase. For a given production schedule, economically optimal production during a production phase and an optimal grade transition between production phases have to be established by properly setting the control variables of the process. Typical control variables are the flow ratio of hydrogen to monomer or the flow rate of an agent modifying stereospecificity. For a fixed production schedule, this objective can be cast into a so-called multistage dynamic optimization problem to determine the time-varying profiles of the control variables to maximize an economical profit function and to meet quality and production constraints. The formulation of this optimization problem will be discussed in Section 3.2.

The optimization of the production is, however, also subject to decision making. Most importantly, it has to reflect market demand to be able to satisfy the requested amounts of grades to be produced until a certain due date with a given specification on the quality indices. Often, there is a priority of satisfying the

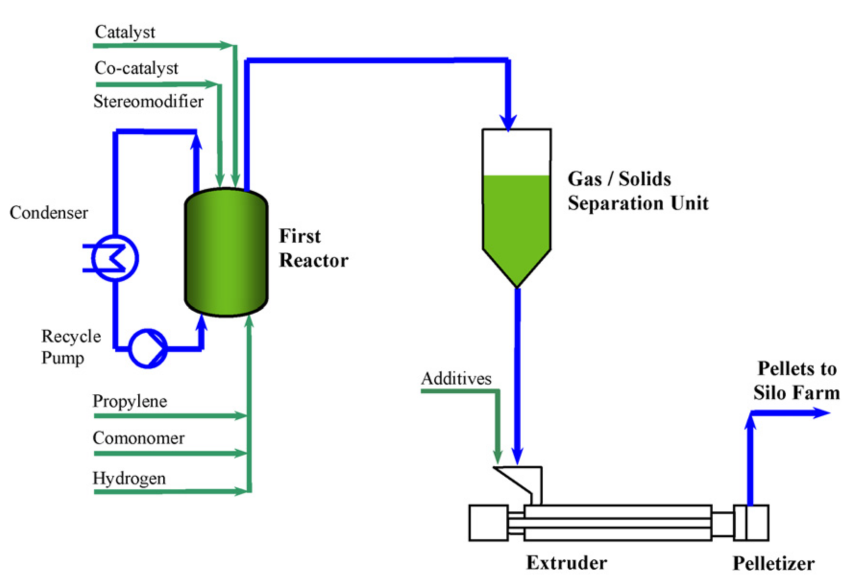

Fig. 1. Simplified flowsheet of the polymerization process.

demand of a certain customer in addition. The market demand changes continuously giving rise to the need for adjusting the schedule in real-time (Castro et al., 2004). The schedule should not only reflect market demand but also the economics of the production. Hence, the sequence of the grades produced as well as the transition between grades should be chosen to achieve the most economical way of production. In particular, the amount of off-spec material, the cost of the raw materials as well as the production time has to be considered simultaneously. Obviously, the schedule and the transition between different production phases are interrelated. Rather, the economics of producing a given set of grades, given amounts before given due dates is determined by both, the schedule as well as the transitions between the production stages. This gives rise to an integrated solution of the scheduling as well as the grade transition problem. A mathematical formulation for this integrated problem will be presented in Sections 3.3 and 3.4 for schedules with and without a consideration of due dates. For simplification, priorities on satisfying the demand of a customer are not considered here.

2.2. Manufacturing problem

In the remainder of this paper we treat a series of case studies in polymer manufacturing, which are similar to those appearing in a real-life polymer production. These case studies are concerned with the determination of the optimal production schedule and grade transitions for a given set of products or orders.

Typically, a production schedule can include up to 20 different products to result in a production plan for the next 5–7 days according to the amount of polymer ordered by the customer. In industry, this procedure is typically performed without truly taking into account the influence of the grade transitions between different grades. The ability to determine the optimal production schedule taking into account the production phases and the grade transitions is of great interest to the polymer production industry.

The integrated scheduling and transition problem is characterized by certain terms which are clarified next for later reference. Production phases and grade transitions will be called production and transition stages, respectively. A grade is defined by the specification of the relevant quality indices. An order refers to a certain amount of polymer satisfying the customer's quality and due date requirements. Hence, an order is referring to a grade but has due amount and due date as additional qualifiers. The due amount refers to the amount that has to be produced and the due date to the date by which production has to be completed to fulfill an order. The term product refers to the material, which is produced during a certain production stage. For further simplification, we will not distinguish between product and order throughout this work. Hence, we tacitly assume that any given order is produced in a single production stage. However, it could make sense from a practical point of view to split and distribute the production of one grade over more stages, when for example the off-spec material produced during transitions may lie within the quality specifications from a possible order, or when due to various reasons the production of an order has to be interrupted and continued later. Hence, splitting and merging products to satisfy the requirements of different orders is not considered here. Obviously, this way the problem complexity is reduced significantly.

2.3. Polymerization reactor model

Due to confidentiality reasons, we cannot explicitly give the mathematical equations describing the polymerization reactor and do not refer to any technical terms that may reveal information with respect to the polymerization technology. The model we are using for the polymerization reactor is part of a more complex process model describing the entire polymerization flowsheet and which has been used in industrial application projects.

A first-principles based modeling approach derives the model including reaction kinetics for the polymerization and equations describing the mass and heat transport phenomena. Our model shares common characteristics with those used in previous studies by McAuley and MacGregor (1992) as well as by Tousain (2002). A broad range of operating conditions can be accommodated by tuning the model parameters by means of nonlinear parameter estimation using available plant data. The polymerization reactor model represents all these characteristics of the process in a mathematical form, in particular their changing influence on the overall operation as changes in process parameters occur.

The performance and accuracy of the mathematical model obtained was verified against plant data and certain physical parameters were modified so that the model shows a good approximated behavior of the real-world process. The model is of medium size and comprises about 80 differential–algebraic equations. Due to the complexity of the polymerization process model, e.g. nonlinearities and stiffness, its numerical solution is a critical issue and an advanced and efficient simulation and optimization tool is required.

3. Mathematical problem formulations

3.1. Fundamentals

Let the following set of differential–algebraic equations (DAE) of an index not greater than one describe the polymerization reactor:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x, z, u, p, t), \quad t \in [t_0, t_{\mathrm{f}}], \tag{1}$$

$$0 = g(x, z, u, p, t), \quad t \in [t_0, t_{\mathrm{f}}], \tag{2}$$

$$x(t_0) = x_0. \tag{3}$$

Eqs. (1) and (2) represent the differential and algebraic model equations, respectively. The vector of differential state variables is represented by x and x_0 is the initial value of the state at time t_0. The algebraic state and control variables contained in Eqs. (1) and (2) are denoted with z and u, respectively. Moreover, p denotes time-invariant model and design parameters. The state and output variables can be calculated on the given time horizon

$t \in [t_0, t_f]$ by solving the DAE model (1)–(2) for given initial conditions x_0 (cf. Eq. (3)), control variables $u(t)$ and parameters p.

Examples for the algebraic variables of the polymerization process model include the quality variable qv_n where $n \in Q = \{1, \ldots, n_q\}$ denotes the quality variable index and n_q the total number of quality variables. The raw material feed flow rate $\dot{m}_{\mathrm{raw}}$ and the amount of material produced m are also included in the vector of algebraic variables. The control variables $u_n(t)$, $n \in C = \{1, \ldots, n_c\}$ are used to manipulate the production in order to achieve the desired product quality.

3.2. Grade transitions for a fixed schedule

In a first scenario, we assume that the schedule is known, i.e. the sequence of alternating production and transition stages for the production of a given set of products (or orders) is fixed. Fig. 2 illustrates the situation for a simple scenario of three production stages (product 1–3), which are connected by two transition stages. This figure also displays the quality bands, which are different for each production stage in general. Most of the material produced during the transition stages does not satisfy the quality requirements. Such off-spec product is of reduced or no economic value and therefore deteriorates the economics of the production considerably. In this section, a multistage dynamic optimization problem (see Leineweber, Bauer, Bock, & Schlöder, 2003 and Vassiliadis, Sargent, & Pantelides, 1994) is formulated on the basis of the model (1)–(3) to address optimal production of a given set of orders assuming a fixed schedule.

Let s denote the stage index and n_s the total number of stages $s \in K = \{1, \ldots, n_s\}$. As can be seen in Fig. 2, a production stage is denoted by odd $s \in U = \{1,3,5, \ldots, n_s\}$ and a transition stage is denoted by even $s \in V = \{2,4,6, \ldots, n_s - 1\}$. As a result, the total production time is divided into n_s stages. The switching time from a production to a transition stage and vice versa is denoted as t_s. The duration of a stage $\Delta t_s = t_s - t_{s-1}$ is treated as a time invariant parameter by introducing a transformation of the time coordinate (see e.g. Büskens (1993)). With these definitions, the multistage model can be formulated as

$$\frac{\mathrm{d}x_s}{\mathrm{d}t} = f_s(x_s, z_s, u_s, p, t), \quad t \in [t_{s-1}, t_s], \quad \forall s \in K, \tag{4}$$

$$0 = g_s(x_s, z_s, u_s, p, t), \quad t \in [t_{s-1}, t_s], \quad \forall s \in K, \tag{5}$$

$$x_1(t_0) = x_0, \qquad x_s(t_{s-1}) = x_{s-1}(t_{s-1}), \quad \forall s \in K. \tag{6}$$

Eq. (6) refers to the initial conditions of the model valid during stage s. The initial states $x_s(t_{s-1})$ on stage s are coupled to the final value of the state of the previous stage $s-1$. Hence, a continuity condition, the so-called stage transition condition is formulated in Eq. (6) to match the states of subsequent stages at the switching points. Eqs. (4)–(6) form a multistage simulation model for given initial conditions, time-invariant parameters p_s and trajectories of the control variables u_s on all stages $s \in K$.

For optimization purposes, the initial conditions x_0 and parameters p are assumed to be given and the control variables $u(t)$ are considered as degrees of freedom to be determined to optimize some objective function. There are typically multiple objectives to be simultaneously satisfied during plant operation including the minimization of total production time, of raw material consumption or of the amount of off-spec material produced during a transition. This multi-criteria objective is expressed by the functional:

$$\phi = W_T t_{n_s} + W_{\mathrm{raw}} \sum_{s \in K} M_{\mathrm{raw},s}(t_s) + W_{\mathrm{off}} \sum_{s \in V} M_{\mathrm{off},s}(t_s) \tag{7}$$

a weighted sum of the individual criteria with weights W_{T}, W_{raw}, and W_{eff} to avoid the computation of the Pareto optimal surface. $M_{\mathrm{raw},s}(t_s)$ refers to the amount of raw material consumed in stage s. This quantity is computed from integrating the raw material feed flow rates $\dot{m}_{\mathrm{raw},s}$ from t_{s-1} to t_s. The off-spec amount $M_{\mathrm{off},s}(t_s)$ is computed by summing the amount of polymer $P_s(t_s)$ produced during all transitions stages:

$$M_{\mathrm{off},s} = \sum_{s \in V} P_s(t_s). \tag{8}$$

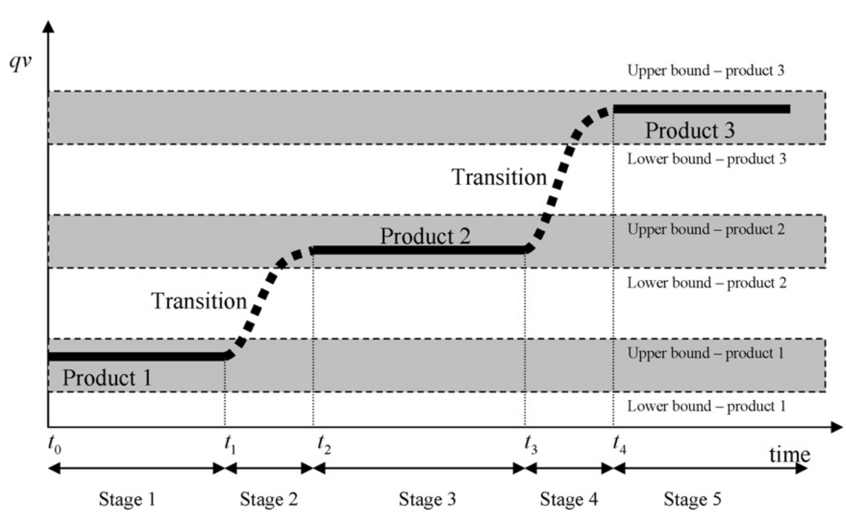

Fig. 2. An example of a production schedule for three polymer products.

In order to meet the customers' product specifications, we have to introduce product quality path constraints during every stage and endpoint constraints on the amount of material produced at the end of every stage. Product quality constraints can be written for any grade g produced on stage s to satisfy:

$$B_{g,\mathrm{low}}^{\mathrm{qv}_n} \leq qv_n^s(t) \leq B_{g,\mathrm{up}}^{\mathrm{qv}_n}, \quad t \in [t_{s-1}, t_s], \quad \forall s \in U, \quad \forall n \in Q. \tag{9}$$

The constants $B_{g,\mathrm{low}}^{\mathrm{qv}_n}$ and $B_{g,\mathrm{up}}^{\mathrm{qv}_n}$ represent the lower and upper bounds for all $n \in \{1, \ldots, n_\mathrm{q}\}$ quality variables for the corresponding grade $g \in G = \{1, \ldots, n_g\}$ produced during production stage s. Endpoint constraints enforce the requested amount of material A_g of grade g produced during a production stage s:

$$P_s(t_s) \geq A_g, \quad \forall g \in G, \quad \forall s \in U. \tag{10}$$

Such constraints do not exist for transition stages, where the amount of off-spec material is supposed to be minimized as enforced by the objective function defined in Eq. (7). While path constraints do not have to be enforced for the quality variables during the transition stage $s \in V$, the following end point constraints are considered to ensure a feasible initial state in the reactor at the beginning of the subsequent production stage:

$$B_{g,\mathrm{low}}^{\mathrm{qv}_n} \leq \mathrm{qv}_n^s(t_s) \leq B_{g,\mathrm{up}}^{\mathrm{qv}_n}, \quad \forall s \in V, \quad \forall n \in Q. \tag{11}$$

Summarizing, the optimization problem can be mathematically expressed as a multistage optimization problem where the objective function shown in Eq. (7) is minimized subject to the DAE model constraints given in Eqs. (4)–(6) and the path and endpoint constraint (8)–(11) if an order defined by grade g and due amount A_g is assigned to every production stage s. The degrees of freedom are the control variables $u_n(t)$ and the optimized production times for each stage Δt_s. The solution of this multistage dynamic optimization problem fixes the optimal transitions for a given set of grades and for a fixed production sequence. It should be noted that the differences of this formulation to the one used by Flores-Tlacuahuac and Grossmann (2006) are substantial. We do not ask for a production wheel nor do we require consistent steady-state control and state variable setpoints. Furthermore, the transition times are decision variables to be determined simultaneously with the control variables and the sequences of the grades.

3.3. Integrated scheduling and grade transition without due dates

In this subsection, the optimization problem is extended to account for the determination of the optimal production sequence. A disjunctive optimization model is developed to facilitate the assignments of orders to a stage s. An order is assumed to comprise grade and due amount information, no due dates are assumed to be included yet. The assignment of orders to production stages is supposed to determine the most favorable production schedule as a result of the optimization. Obviously, such an assignment process requires discrete decisions to match a certain order by the manufacturing process on a certain stage. Such a task is combinatorial in nature. Care has therefore to be taken to come up with a suitable model, which limits combinatorial complexity to the extent possible. According to our assumption of not splitting and distributing orders over more than one stage or merging the produced amount to satisfy the demand of one order, no discrete events can occur during a production or transition stage. This simplification of the optimization model is required in order to limit the complexity of the problem. All discrete decisions take place at the stage boundaries.

Based on this simplifying assumption, we introduce a set of Boolean variables:

$$X_{g,s} \in \{\mathrm{True}, \ \mathrm{False}\}, \quad \forall g \in G, \quad \forall s \in V, \tag{12}$$

in order to mathematically express if a certain grade g is produced on a certain production stage s. If a grade g is produced on stage s, we define $X_{g,s} = \mathrm{True}$.

To model the discrete decisions, a set of logical constraints is added to the multistage model (4)–(11) derived in the last section. These equations extend the optimization problem to a MIDO problem. We choose to represent the discrete decisions by logical constraints involving disjunctions to implicitly specify all possible production schedules. The choice of which product shall be produced on which stage is mathematically expressed by employing a suitable concept of modeling conditional equations. We have two different sets of disjunctive terms s and g which are related to the two-dimensional Boolean decision variable $X_{g,s}$:

$$\vee_{s \in U} \begin{bmatrix} X_{g,s} \\ B_{\mathrm{low},g}^{\mathrm{qv}_n} \leq \mathrm{qv}_n^s(t) \leq B_{\mathrm{up},g}^{\mathrm{qv}_n} \\ P_s(t_s) \geq A_g \end{bmatrix},$$

$$\forall g \in G, \quad \forall n \in Q, \quad t \in [t_{s-1}, t_s]. \tag{13}$$

The disjunction expresses that if a grade g is produced on stage s, i.e. if $X_{g,s} = \mathrm{True}$, the quality variables qv_n and the amount of material produced P_s are constrained within and at the end of production stage s according to the order specifications. These constraints are identical to (9)–(11), but are now formulated in a conditional form, expressed by disjunctions. The disjunctions allow to include or exclude the constraints in the problem formulation to reflect the decision of assigning an order to a stage. No disjunctions have to be stated for the transition stages, since these related decisions are implicitly fixed by the alternating transition-production stage sequence as soon as the decisions on the production stages are taken.

The combinatorial complexity of the integrated scheduling and grade optimization problem obviously increases with the number of Boolean variables and disjunctive terms. For example, if we have nine different products, we end up with 17 stages (nine production stages and eight transition stages) and 81 Boolean variables. The number of possible combinations (production sequences) is $9! = 362{,}880$. In order to make sure that no undesirable combinations occur during optimization, we introduce the logic constraints:

$$X_{g,1} \veebar X_{g,3} \veebar X_{g,5} \veebar \ldots \veebar X_{g,n_s}, \quad \forall g \in G, \tag{14}$$

$$X_{1,s} \veebar X_{2,s} \veebar X_{3,s} \veebar \ldots \veebar X_{n_g,s}, \quad \forall s \in U. \tag{15}$$

These logic constraints enforce that once a grade is being produced within one stage, it cannot be produced within one of the other stages and that the production of more than one grade within one production stage is excluded from the set of operational options.

The resulting mixed-logic dynamic optimization problem (MLDO) given by Eqs. (4)–(11) can be reformulated as a MIDO problem using either a big-M or a convex hull reformulation of the disjunctions (Oldenburg & Marquardt, 2005; Oldenburg & Marquardt, submitted). In this work, a big-M reformulation approach is employed. First, the Boolean variables $X_{g,s}$ are replaced by binary variables $X^*_{g,s} \in \{0, 1\}$. Then, the disjunctions (13) are converted into the following set of inequalities:

$$\mathrm{qv}_n^{s,g}(t) \le B^{\mathrm{qv}_n}_{\mathrm{up},g} + M(1 - X^*_{g,s}),$$
$$\forall g \in G, \quad \forall s \in U, \quad \forall n \in Q, \quad t \in [t_{s-1}, t_s], \tag{16}$$

$$\mathrm{qv}_n^{s,g}(t) \ge B^{\mathrm{qv}_{n1}}_{\mathrm{low},g} - M(1 - X^*_{g,s}), \quad \forall g \in G, \quad \forall s \in U,$$
$$\forall n \in Q, \quad t \in [t_{s-1}, t_s], \tag{17}$$

$$P_s(t_s) \ge A_g - M(1 - X^*_{g,s}), \quad \forall g \in G, \quad \forall s \in U. \tag{18}$$

The value of the constant M has to be chosen large enough to avoid cutting off parts of the feasible solution. The logic constraints (14) and (15) are translated into the binary constraints:

$$\sum_{s \in U} X^*_{g,s} = 1, \quad \forall g \in G, \tag{19}$$

$$\sum_{g \in G} X^*_{g,s} = 1, \quad \forall s \in U, \tag{20}$$

The resulting MIDO problem finally consists of Eqs. (4)–(8) and (16)–(20).

3.4. Accounting for due dates of an order

In the previous subsection, the problem formulation did not account for due dates as part of an order. However, due dates are very common in practice and have to be accounted for in the optimization problem (Nyström et al., 2005). The problem formulation above is extended here to account for due dates.

For this purpose, we need to calculate the time when the production of a certain grade has to end. To achieve this, we formulate the following disjunction:

$$\vee_{s \in U} \begin{bmatrix} X_{g,s} \\ \sum_{z \in U} t_{f,z} \ge D_g \end{bmatrix}, \quad \forall g \in G, \tag{21}$$

where D_g denotes the due date of grade g.

In order to limit the large number of possible combinations, the logical constraints (14) and (15) need to be taken into account, too. For the numerical solution, they are transformed into the binary constraints (19) and (20) and the logic constraint (21) is converted into the corresponding binary constraint by using a big-M formulation:

$$\sum_{z \in U} t_{f,z} \le D_g + M(1 - X^*_{g,s}), \quad \forall g \in G, \quad \forall s \in U. \tag{22}$$

$X^*_{g,s} \in \{0, 1\}$ represents binary variables and replace the Boolean variables $X_{g,s}$ from Eq. (21) as explained before. Eq. (22) is used to calculate the total production time until a certain grade is produced on a certain stage s.

4. Numerical solution method

The infinite-dimensional optimization problem (cf. Eqs. (4)–(12), (20)–(22)) is approximated by a finite-dimensional optimization problem using a combined discretization scheme (Oldenburg & Marquardt, 2005; Oldenburg & Marquardt, submitted; Oldenburg, Marquardt, Heinz, & Leineweber, 2002; Oldenburg, Marquardt, Heinz, & Leineweber, 2003) based on direct single and multiple shooting. The resulting vector of discretized decision variables collects the discretized control variables u_s, time-invariant parameters p_s, the initial values of all state variables x_s and the stage durations Δt_s on each stage. Together with the binary variables, the discretized dynamic optimization problem results in a mixed-integer nonlinear programming problem (MINLP). The chosen modeling and solution approach is well suited for the integrated scheduling and dynamic optimization problem addressed in this contribution which is characterized by (i) mixed discrete-continuous dynamics and (ii) a strongly nonlinear and stiff industrial DAE process model.

The solution procedure is based on an implicit treatment of the dynamic model constraints, i.e. the differential and algebraic state variable profiles for each stage are obtained by a numerical integrator. The resulting MINLP problem is solved using a decomposition method, the so-called outer approximation (OA) algorithm by Duran and Grossman (1986) with extensions (Viswanathan & Grossmann, 1990) to account for nonconvexity. The algorithm bounds the solution from above and from below by alternating between a nonlinear programming (NLP) phase to fix the continuous variables and a mixed-integer linear programming (MILP) phase to fix the integer variables. If the overall optimization problem is convex, the difference between the minimum of all upper bounds and the non-decreasing lower bound will be less than or equal to a specified tolerance after a certain number of iterations and the optimization stops. The problem treated in this work, however, constitutes a nonconvex problem due to the nonlinearity of the process dynamics (Nyström et al., 2005). Thus, the heuristic augmented penalty (AP) extension of the OA method proposed by Viswanathan and Grossmann (1990) is applied. With this method, no guarantee can be given that the global minimum or even a good local minimum is found in a finite number of iteration. Experience with applications from various areas has, however, shown that satisfactory results are obtained in many cases. For a variety of examples, we refer e.g. to Oldenburg et al. (2002, 2003) and Oldenburg and Marquardt (submitted) or Busch et al. (2005, 2007). This experience is supported by the optimization results

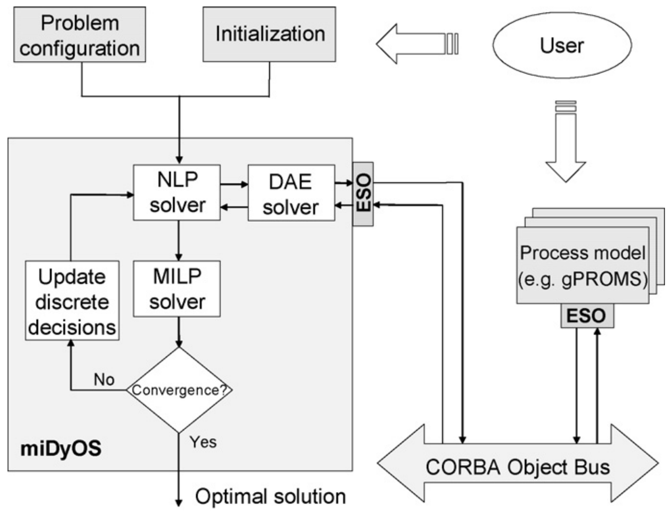

Fig. 3. Software architecture and computational flow diagram of miDyOS.

presented in Section 5. Nevertheless, the availability of global solution methods, which are unfortunately not yet capable of solving problems of the present size, are highly desirable.

For solving the case study problem in this paper, the software tool DyOS (Brendel, Oldenburg, Schlegel, & Stockmann, 2003; Schlegel, Stockmann, Binder, & Marquardt, 2005) developed at Lehrstuhl für Prozesstechnik, RWTH Aachen University, is used. For MIDO problems, miDyOS (the mixed-integer extension of DyOS) implements a combined direct single and multiple shooting method. miDyOS applies a decomposition strategy based on the OA method. As shown in Fig. 3, miDyOS incorporates an interface to CPLEX (ILOG, 2002), which is used as the MILP solver for the master subproblems. Furthermore, NPSOL (Gill, 1998) and SNOPT (Gill, Murray, & Saunders, 1998) are employed as NLP solvers for the primal subproblems within the miDyOS optimization framework. Within miDyOS the dynamic model equations are provided by the user through the implementation of the process model in gPROMS (2002) or any other modeling environment which is compliant to the CAPE-OPEN standard. A Common Object Request Broker Architecture (CORBA) establishes the connection between the model server (gPROMS) and the optimizer (miDyOS). For this purpose, the process model equations are transformed into a so-called equation set object (ESO) defined in Keeping and Pantelides (1999).

5. Numerical results

In this section we present the numerical results obtained for a case study with six production grades. The difficulty of the optimization problem is gradually increased, starting with a fixed production schedule, followed by calculating the production sequence and finally accounting for due dates.

5.1. Fixed production schedule

We consider the fixed production sequence 1–6, i.e. grade 1 is produced first, grade 2 is produced second, and so on with a transition stage between two different production stages. The grade specifications are listed in Table 1. The objective function is defined according to Eq. (7).

Table 1
Grade specifications for a six grades production campaign

Grade	$B^{\mathrm{MI}}_{\mathrm{low}}$ (g/10 min)	$B^{\mathrm{MI}}_{\mathrm{up}}$ (g/10 min)	$B^{\mathrm{SSP}}_{\mathrm{low}}$	$B^{\mathrm{SSP}}_{\mathrm{up}}$	A (tons)
1	0.2	0.4	90	110	60
2	0.7	0.9	190	210	60
3	1.2	1.4	290	310	60
4	0.7	0.9	90	110	60
5	1.2	1.4	190	210	60
6	0.7	0.9	290	310	60

The results obtained with miDyOS are presented in Figs. 4–7. The quality variables MI and SSP, as well the control variables are bounded from below and above. The lower and upper bounds are drawn with dashed lines. Vertical dashed lines delimit the beginning and the end of a transition stage.

The initial values x_0 of the states at $t_0 = 0$ for the first production stage have been chosen such that the values of MI and SSP lie within the lower and upper bounds corresponding to this grade. The same values have been used as initial guesses for the initial values on the remaining stages at $t_1, t_2, \ldots, t_{s-1}$. The initial guesses for the durations Δt_s for all stages are chosen based on available process know-how. The optimization yields that these values lie within in a range of ±15% of the optimized value. This initialization is kept und used for all case studies presented in the sequel.

For computational tests, a Pentium IV with a 2.0 GHz processor has been used. The computational time required to find the optimal solution for the example dynamic optimization problem is about 120 s. This example clearly shows the performance of the multistage algorithm and the ability of the solver of finding the optimal profile for the control variables for a given production sequence that in reality lasts for about 3 days.

It can be observed that continuity was enforced for both quality variables between all the stages. Tighter bounds on the control variables can lead to a slightly worse optimization result and to a small increase of the computational burden. In this case study we do not employ realistic bounds on the control variables for not revealing the real transition durations due to confidentiality reasons. It has to be mentioned that all fast grade transitions that can be seen in Fig. 4 cannot be achieved in a real plant due to necessary restrictions of the control variables for safety reasons.

5.2. Integrated scheduling and grade transition without due dates

As explained before, miDyOS starts solving first the NLP subproblem for a fixed initial set of binary variables, which is used for initialization of the problem. We start in this example with the initial production sequence 1–6 as an initial guess. All initials are taken from the converged solution presented in Section 5.1.

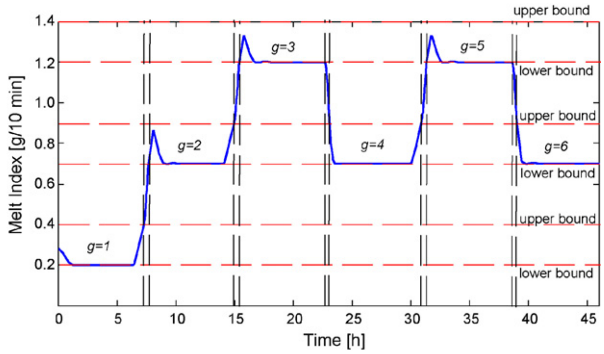

Fig. 4. Production campaign with fixed schedule, quality variable MI.

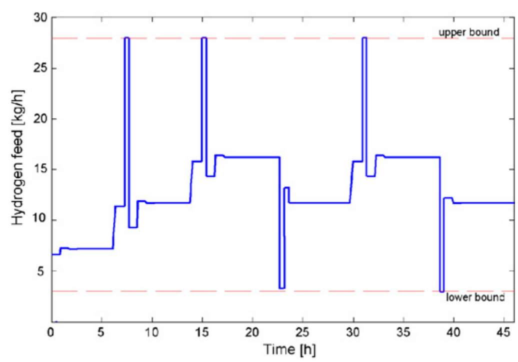

Fig. 5. Production campaign with fixed schedule, control variable hydrogen feed.

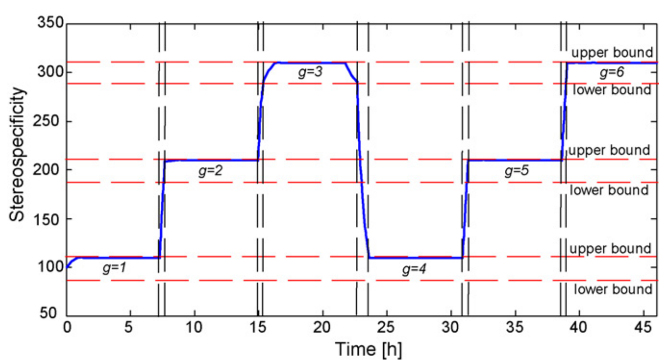

Fig. 6. Production campaign with fixed schedule, quality variable SSP.

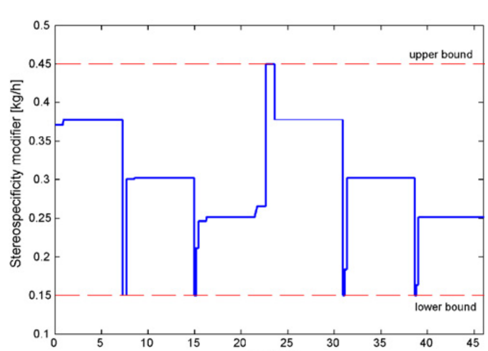

Fig. 7. Production campaign with fixed schedule, control variable stereospecificity modifier.

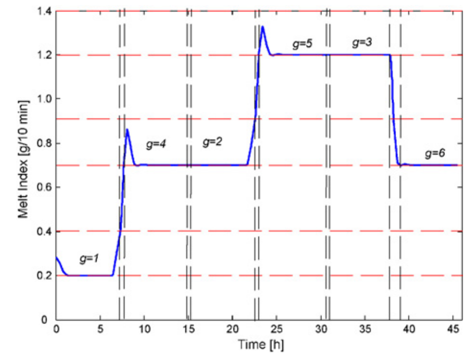

Fig. 8. Integrated scheduling and grade transition, output variable MI.

By adding Boolean variables, disjunctions and propositional logic constraints to the dynamic optimization problem, we can determine the optimal sequence in which all six products should be produced such that all quality constraints are met. miDyOS starts iterating between the NLP and the MILP problem and stops as soon as there is no improvement in two successive primal solutions. After the optimization process stops, the best sequence is naturally that one, for which the corresponding NLP problem has the smallest value for the objective function. Moreover, the user can specify the maximum and the minimum number of major iterations. Hence, the user can adjust the search according to the main two possibilities of either finding an acceptable and feasible solution fast or to determine a local minimum, which is more likely to be closer to the global minimum.

In this example, the solver stops after four iterations and finds the optimal production sequence as being 1–4–2–5–3–6.

The quality variables and the control variables for the best production sequence are plotted against time in Figs. 8–11. The lower and upper bounds are drawn with dashed lines.

The results obtained with the OA algorithm with augmented penalty extension are summarized in Table 2. The algorithm stops after four major iterations and the optimal solution with sequence 1–4–2–5–3–6 is found in the third iteration using about 48 min of total CPU time on a Pentium IV with a 2.0 GHz processor. The CPU time required for solving the NLP problems is substantially higher than that required for solving the MILP problems in each iteration.

Table 2
Optimization results obtained with an OA–AP algorithm for a production campaign with six grades and without due date constraints

	Iteration			
	#1	#2	#3	#4
Primal problem				
Objective	23.47	23.38	23.13*	23.24
Solution time (s)	131.26	793.42	745.92	767.25
Master problem				
Objective	22.59	23.29	510.13	960.45
Solution time (s)	33.66	32.94	127.86	223.63

* Indicates optimal solution.

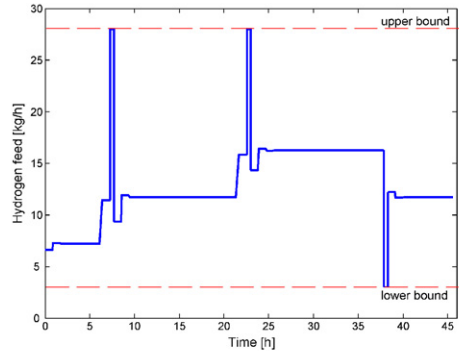

Fig. 9. Integrated scheduling and grade transition, control variable hydrogen feed.

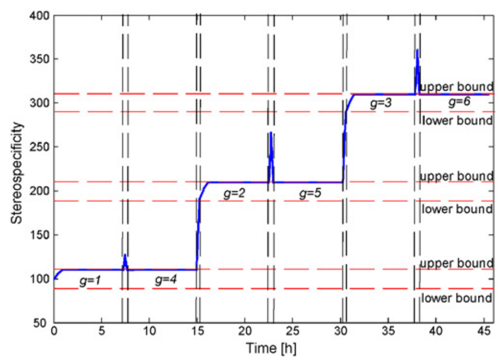

Fig. 10. Integrated scheduling and grade transition, output variable SSP.

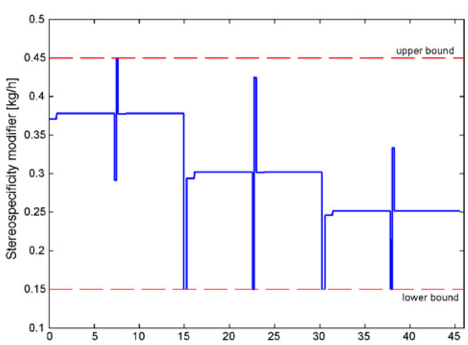

Fig. 11. Integrated scheduling and grade transition, control variable stereospecificity modifier.

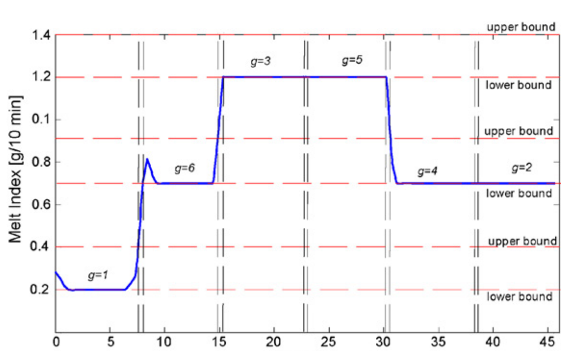

Fig. 12. Integrated scheduling and grade transition with due date, output variable MI.

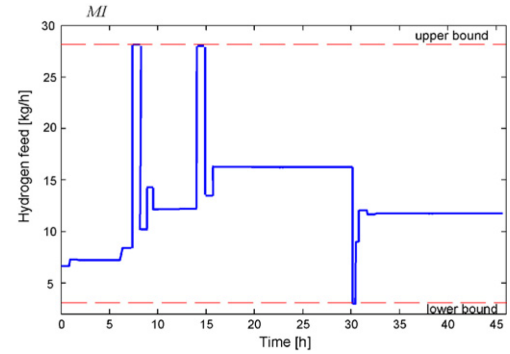

Fig. 13. Integrated scheduling and grade transition with due date, control variable hydrogen feed.

5.3. *Integrated scheduling and grade transition optimization with due dates*

In this section, we present the results for the case study that an order comprises grade, due amount and due dates information. For illustration purposes, we enforce a due date constraint for grade 3, i.e. $D_3 = 25$ h in this example.

For certain combinations of binary variables, it may happen that no feasible point is found for the primal problem. This may appear for example, in the case when grade 3 is assigned to a stage, whose production end-time is greater than the due-date constraint that has been set active by the binary variable $X^*_{g,s}$. In this case, miDyOS generates automatically an integer cut and the current combination of binary variables is excluded for the next MILP problems. For further details we refer to the DyOS users' guide.

Figs. 12–15 show the results obtained if a due-date constraint is enforced for grade 3. The optimal production sequence is 1–6–3–5–4–2 and is found after six iterations. As expected, grade 3 is produced during one of the first three production stages. All other combinations of binary variables requesting grade 3 to be produced on the remaining production stages, render the optimization problems to become infeasible.

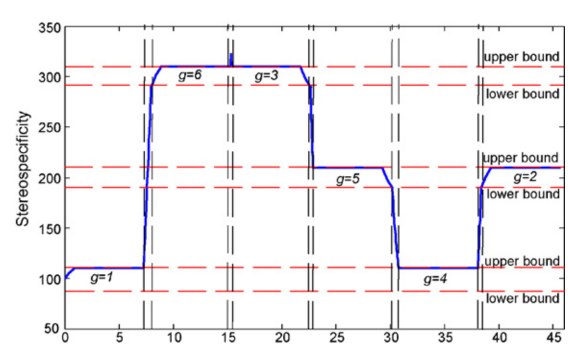

Fig. 14. Integrated scheduling and grade transition with due date, output variable SSP.

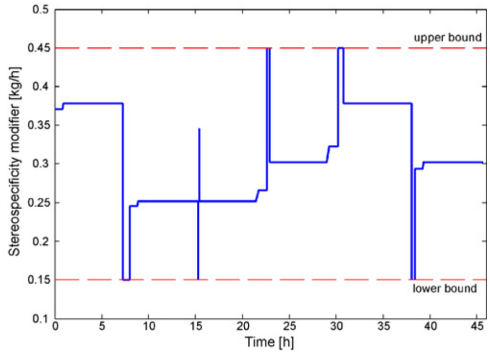

Fig. 15. Integrated scheduling and grade transition with due date, control variable stereospecificity modifier.

The results obtained with the OA–AP algorithm for the six grades production campaign with a due date constraint are summarized in Table 3. Again, using a Pentium IV computer with a 2.0 GHz processor, the total CPU time amounts to about 73 min. Of course, the number of OA primal problems that has been solved is higher than six. In this case, we have six major iterations with feasible NLP problems, and six with infeasible NLP problems. For certain combinations of binary variables determined after solving the OA master problem from the previous major iteration, the NLP subproblems are infeasible. In this case, the MIDO algorithm is not stopped on the basis of infeasible primal problems. Instead, the current combination of binary variables that resulted in the infeasible primal problem has been excluded within the subsequent master problem by an integer cut, and a new set of binaries is generated. If the NLP problem is feasible but the requested accuracy cannot be achieved, then the entire optimization procedure stops and no MILP problem is generated. This can happen for example if the model is badly scaled, or if the tolerances are not set appropriately. Consequently, only the results for the feasible primal problems and the respective MILP problems are shown in Table 3. Naturally, the due date constraint $D_3 = 25$ is fulfilled for all sets of binaries for which the primal subproblems were found to be feasible until the algorithm stopped. Of course, there are other aspects that may lead to infeasibilities for a certain primal subproblem, like a bad initial guess for the process model. But this is not the case here, since the algorithm was tested for the same optimization problem and initial guess, but without due dates and no infeasible primal sub-problems arose.

5.4. Discussion of the results

In summary, it can be concluded that optimizing the sequence in which the products are produced can save a significant amount of production time and raw material. It has been observed that based on the optimal production sequence, the same number of grades can be produced, with the same due amounts and quality specifications, but in a total production time of 45 min less in comparison with that needed for the initial sequence 1–6. The main difference results however from the amount of off-spec material that is produced during all transition stages. As a matter of fact, the optimal solution shows only small changes in the quality variables as compared to the fixed sequence.

The solution approach has also been applied for solving optimization problems with a larger number of different polymer grades. The computational burden increases in this case quite rapidly, especially for solving the master problems. To get a rough impression, 110 CPU min were required to determine an optimal schedule for a nine grade production campaign without due date constraints. Note that for optimization problems with a larger number of grades, rescheduling and uncertainty aspects – which are not addressed in this work – become increasingly important.

The computing time expectedly increases with the complexity of the problem from 2 min for the fixed schedule to 48 min for integrated scheduling and grade transition without due date and to 73 min for integrated scheduling and grade transition with a due date. The increase for the problem might be surprising, since the number of discrete states is reduced by adding the constraint. However, enforcing the due date constraint results in continuous NLP problems which are more difficult to solve. We have observed a larger number of iterations where the NLP problem resulted in optimal solutions with objective values that were very close. The total CPU time depends on the sequence of iterations and the choice of the stopping criterion, and in particular on the nature of the optimization problem. Still, the computing times are very moderate. In fact, a real-time implementation of the integrated scheduling and transition optimization strategy on a receding horizon is already feasible for the case study treated in this paper.

Table 3
Optimization results obtained with an OA–AP algorithm for a production campaign with six grades and with due date constraints

	Iteration							
	#1	#2	#3	#4, #5	#6	#7, #8, #9, #10	#11	#12
Primal problem								
Objective	23.46	23.38	23.36	Infeasible	23.16	Infeasible	23.14*	23.29
Solution time (s)	104.48	214.64	215.03	420.50	632.98	950.80	324.74	463.20
Master problem								
Objective (including slacks terms)	22.65	25.01	968.23	–	1881.49		2498.84	3469.31
Solution time (s)	20.34	29.13	114.58	–	174.76		241.54	447.54

* Indicates optimal solution.

6. Conclusions

A novel approach for modeling and solving an integrated scheduling and grade transition problem has been presented. It is based on a rigorous process model of the process system and does not rely on operational plant experience to fix the transition and processing times as it is practice in current scheduling applications. The main focus of this paper is to show that the determination of an optimal sequence of alternating production phases and grade transition phases by means of rigorous mixed-integer dynamic optimization is feasible for a realistic problem taken from polymers manufacturing. The approach can be expected to evolve into a standard solution method for the scheduling of production campaigns for continuous manufacturing processes, where the explicit consideration of process dynamics is desirable. In fact, even reactive scheduling in real-time requiring an implementation of the methodology on a receding horizon becomes feasible. Such a case study has been reported by Busch et al. (2007) recently in the context of wastewater treatment plants. The proposed methodology also qualifies for other dynamic optimization problems where discontinuities or discrete events might appear (Oldenburg & Marquardt, 2005). The way we have formulated and solved the mixed-integer dynamic optimization problem was experienced to be robust and efficient.

The approach presented in this article has proven its importance in conjunction with a real-life industrial problem. The study has demonstrated the potential of improving economic performance of industrial polymer production by incorporating optimal grade transitions into a scheduling formulation.

In current work, the scheduling problem is extended to the case where flowsheet changes are implemented depending on the ordered products. For example, in many polymerization plants, certain products such copolymers require additional process units affecting the overall production schedule. In those cases such additional pieces of equipment have to be included or removed from the problem. Since the dynamic model changes dramatically from one stage to the next, a higher level of combinatorial and computational complexity has to be expected.

Acknowledgements

The European Union is gratefully acknowledged for the support of Adrian Prata under the Marie Curie Fellowship, contract No. HPMI-CT-2001-00138. Furthermore, we thank Rasmus Nyström for fruitful discussions and for reviewing the manuscript.

References

Brendel, M., Oldenburg, J., Schlegel, M., & Stockmann, K. (2003). *DyOS User's Guide Version 2.1. Lehrstuhl für Prozesstechnik*. RWTH Aachen University.

Busch, J., Santos, M., Oldenburg, J., Cruse, A., & Marquardt, W. (2005). A framework for the mixed integer dynamic optimisation of waste water treatment plants using scenario-dependent optimal control. In L. Puigjaner (Ed.), *European Symposium on Computer Aided Process Engineering, Vol. 15* (pp. 955–960). Elsevier.

Busch, J., Oldenburg, J., Santos, M., Cruse, A., & Marquardt, W. (2007). Dynamic predictive scheduling of operational strategies for continuous processes using mixed-logic dynamic optimization. *Computers and Chemical Engineering*, *31*, 574–587.

Büskens, C. (1993). Optimierungsmethoden und Sensitivitätsanalyse für optimale Steuerprozesse mit Steuer- und Zustandsbeschränkungen. PhD Thesis, Westfälische Wilhelms Universität Münster, in German.

Castro, P. M., Barbosa-Póvoa, A. P., Matos, H. A., & Novais, A. Q. (2004). Simple continuous-time formulation for short-term scheduling of batch and continuous processes. *Industrial and Engineering Chemistry Research*, *43*, 105–118.

Chatzidoukas, C., Kiparissides, C., Perkins, J. D., & Pistikopoulos, E. N. (2003). Optimal grade transition campaign scheduling in a gas-phase polyolefin FBR using mixed integer dynamic optimization. In A. Kraslawski & I. Turunen (Eds.), *Proceedings of the European Symposium on Computer Aided Process Engineering, Vol. 13* (pp. 71–77). Elsevier.

Chatzidoukas, C., Perkins, J. D., Pistikopoulos, E. N., & Kiparissides, C. (2003). Optimal grade transition and selection of closed-loop controllers in gas-phase olefin polymerization fluidized bed reactor. *Chemical Engineering Science*, *58*, 3643–3658.

Duran, M., & Grossman, I. E. (1986). A mixed-integer nonlinear programming algorithm for process systems synthesis. *AIChE Journal*, *32*(4), 592–606.

Flores-Tlacuahuac, A., & Grossmann, I. E. (2006). Simultaneous cyclic scheduling and control of a multiproduct CSTR. *Industrial and Engineering Chemistry Research*, *27*, 6698–6712.

Floudas, C. A., & Lin, X. X. (2004). Continous-time versus discrete-time approaches for scheduling of chemical processes: A review. *Computers and Chemical Engineering*, *28*, 2109–2129.

Floudas, C. A., & Lin, X. X. (2005). Mixed-integer linear programming in process scheduling. Modeling, algorithms and applications. *Annals of Operations Research*, *139*, 131–162.

Gallestey, E., Stohert, A., Castagnolli, D., Ferrari-Trecate, D., & Morari, M. (2003). Using model predictive control and hybrid systems for optimal scheduling of industrial processes. *at-Automatisierungstechnik*, *51*(6), 285–293.

Gill, P. E. (1998). User's guide for NPSOL 5.0: A Fortran package for nonlinear programming, Technical Report SOL, pp. 1–44.

Gill, P. E., Murray, W., & Saunders, M. A. (1998). SNOPT: An SQP algorithm for large-scale constrained optimization, Technical Report. Stanford University, USA.

gPROMS. gPROMS User Guide (Release 2.1.1). Process Systems Enterprise Ltd., London, UK, 2002.

Grossmann, I. E. (2002). Review of nonlinear mixed-integer and disjunctive programming techniques. *Optimization and Engineering*, *3*, 227–252.

ILOG CPLEX 7.5, User's Manual, Ilog, Inc., France, 2002.

Joly, M., & Pinto, J. M. (2003). Mixed-Integer programming techniques for the scheduling of fuel oil and asphalt production. *Chemical Engineering Research and Design*, *81*, 427–447.

Kadam, J., & Marquardt, W. (2004). Sensitivity-based updates in closed-loop dynamic optimization. In *Proceeding of the DYCOPS-7*.

Kadam, J., Srinivasan, B., Bonvin, D., & Marquardt, W. (2007). Optimal grade transition in industrial polymerization processes via NCO tracking. *AIChE Journal*, *53*(3), 627–639.

Keeping, B., & Pantelides, C. C. (1999). Cape Open WP4.1 Numerical solvers open interface specification draft. CO-NUMR-EL-03, pp. 357–369.

Kondili, E., Pantelides, C. C., & Sargent, R. (1993). A general algorithm for short-term scheduling of batch operations—I. MILP formulation. *Computers and Chemical Engineering*, *17*, 211–227.

Leineweber, D. B., Bauer, I., Bock, H. G., & Schlöder, J. P. (2003). An efficient multiple shooting based reduced SQP strategy for large-scale dynamic process optimisation. Part I: Theoretical aspects. *Computers and Chemical Engineering*, *27*(2), 157–166.

McAuley, K. B., & MacGregor, J. F. (1992). Optimal grade transitions in a gas phase polyethylene reactor. *AIChE Journal*, *38*(10), 1564–1576.

Mendez, C. A., Cerda, J., & Grossmann, I. E. (2006). State-of-the-art review of optimization methods for short-term scheduling of batch processes. *Computers and Chemical Engineering*, *15*, 913–946.

Nyström, R. H., Franke, R., Harjunkoski, I., & Kroll, A. (2005). Production campaign planning including grade transition sequencing and dynamic optimization. *Computers and Chemical Engineering*, *29*, 2163–2179.

Oldenburg, J., & Marquardt, W. (2005). Optimization of discrete-continuous dynamic systems based on disjunctive programming, 2005. In *Proceedings of the Applied Mathmatical Mechanism (PAMM)—Special Issue: GAMM Annual Meeting 2005* (pp. 51–54).

Oldenburg, J., & Marquardt, W. (submitted). Disjunctive modeling for optimal control of discrete-continuous dynamic systems. *Computers and Chemical Engineering*.

Oldenburg, J., Marquardt, W., Heinz, D., & Leineweber, D. B. (2002). Mixed-logic dynamic optimization applied to configuration and sequencing of batch distillation processes. In J. Grievink & J. van Schijndel (Eds.), *Proceedings of the European Symposium on Computer Aided Process Engineering, Vol. 15* (pp. 283–288). Elsevier.

Oldenburg, J., Marquardt, W., Heinz, D., & Leineweber, D. B. (2003). Mixed-logic dynamic optimization applied to batch distillation process design. *AIChE Journal*, *48*(11), 2900–2917.

Pantelides, C. C. (1994). Unified frameworks for the optimal process planning and scheduling. In *Proceedings of the Second Conference on Foundations of Computer-Aided Operations* (pp. 253–274). New York: Cache Publications.

Schlegel, M., Stockmann, K., Binder, T., & Marquardt, W. (2005). Dynamic optimization using adaptive control vector parameterization. *Computers and Chemical Engineering*, *29*(8), 1731–1751.

Tosukhowong, T., Lee, J. M., Lee, J. H., & Lu, J. H. (2004). An introduction to a dynamic plant-wide optimization strategy for an integrated plant. *Computers and Chemical Engineering*, *29*, 199–208.

Tousain, R. L. (2002). Dynamic Optimization in Business-wide Process Control. PhD thesis, Technical University Delft.

Van Brempt, W., Van Overschee, P., Backx, T., Ludlage, R., Hayot, P., Oostvogels, L., et al. (2003). Economically optimal grade change trajectories: Application on a Dow polystyrene process model. In *Proceedings of the American Control Conference* (pp. 5411–5416).

Vassiliadis, V. S., Sargent, R. W. H., & Pantelides, C. C. (1994). Solution of a class of multistage dynamic optimization problems. 2. Problems with path constraints. *Industrial and Engineering Chemistry Research*, *33*, 2123–2133.

Viswanathan, J., & Grossmann, I. E. (1990). A combined penalty function and outer approximation method for MINLP optimization. *Computers and Chemical Engineering*, *14*(7), 769–782.