Travelling Salesman Problem (TSP) based integration of Planning, Scheduling and optimal Control for Continuous Processes

Vassilis M. Charitopoulos, Vivek Dua, Lazaros G. Papageorgiou*

Department of Chemical Engineering, Centre for Process Systems Engineering, University College London, Torrington Place, London WC1E 7JE, United Kingdom

*<u>**Corresponding Author:**</u> l.papageorgiou@ucl.ac.uk

Advanced decision making in the process industries requires efficient use of information available at different decision levels. Traditionally, planning, scheduling and optimal control problems are solved in a decoupled way, neglecting their strong interdependence. Integrated Planning, Scheduling and optimal Control (iPSC) aims to address this issue. Formulating the iPSC, results in a large scale non-convex Mixed Integer Nonlinear Programming problem. In the present work, we propose a new approach for the iPSC of continuous processes aiming to reduce model and computational complexity. For the planning and scheduling, a Travelling Salesman Problem (TSP) based formulation is employed, where the planning periods are modelled in discrete time while the scheduling within each week is in continuous time. Another feature of the proposed iPSC framework is that backlog, idle production time and multiple customers are introduced. The resulting problem is a Mixed Integer Programming problem and different solution strategies are employed and analysed.

Keywords: process scheduling, planning, dynamic optimisation, enterprise wide optimisation, integration

1 Introduction

Decision making in the process industries is organised in a hierarchical manner and actions are taken in a decentralised fashion with common objectives being the maximisation of profitability, sustainability and safety. Three of the most important functionalities in the chain of command of the industry, involve medium-term planning, production scheduling and advanced process control. Process planning aims to organise the production and meet demands over long time horizons; a planning horizon typically spans from weeks to months and key decisions include the determination of sales, backlog and inventory levels. After the planning decisions have been made, a detailed schedule of production is carried out for each planning week. Production scheduling deals with the optimal resource allocation of the manufacture in greater detail than planning; major decisions include, optimal production and changeover times, sequencing of tasks and so forth. On a lower level in the decision pyramid, advanced process control (APC) is located. APC, involves optimal and model based control strategies that are responsible for the regulation of the process dynamics. For the case of continuous manufacturing systems, such as polymerisation processes, APC aims to secure the optimal operation between transition of different production regimes as well as to maintain the desirable steady state operating conditions. The ever increasing need to maintain profitable and efficient operations in the industry along with recent developments such as parallel computing and more efficient IT infrastructure indicate the dawn of a new era in the way decision making is conducted. Concepts such as enterprise wide optimisation (EWO), smart manufacturing[1] and Industry 4.0[2] underline the need for efficient use of information available among closely related functionalities of the supply chain like medium term planning, production scheduling and optimal control.

1.1 Integration of process operations with control

In Figure 1, the automation pyramid based on the ISA 95 standards is envisaged.

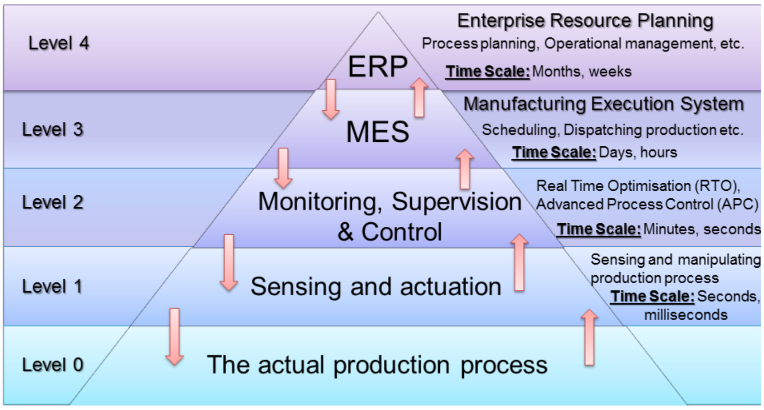


Figure 1: ISA 95 automation pyramid

Based on the ISA 95 standards[3] the levels of hierarchy that we focus on, within this article, are the three top ones. As shown in Figure 1, the three problems involve different time scales and there is information flow, from top to bottom and vice versa. Because of the interdependence existing among these three problems, developing an integrated approach to model and solve the problem is likely to yield better solutions and thus enhance process operations. Indeed, research work from the literature indicate that integration of different decision layers of the automation pyramid can lead to more efficient operations[3–6].

Until recently, the integration was studied from two different perspectives: (i) integration of medium-term planning and scheduling and (ii) integration of scheduling and control. For the problem of integration between planning and scheduling a number of modelling approaches have been proposed in the literature with some researchers formulating the problem in a monolithic way while other researchers employing aggregated modelling techniques or even the development of surrogate models for the problem of scheduling[7]. Regardless of the modelling approach employed, due to the different time scales the computational effort required for the solution of the problem grows rapidly with the length of the planning horizon under consideration. To this effect, solution techniques such as Lagrangean relaxation, rolling horizon and bi-level decomposition have been proposed, to name a few.

Integration of process scheduling and optimal control has been studied recently for both continuous and batch processes[8]. The interactions between scheduling and control can dramatically affect the economically optimal operation of the manufacture, since decisions such as production time, sequencing of tasks and transition time are dependent on the dynamic status of the system. To be more specific, the production rate for a continuous process can be seen as a function of the state variables of the underlying control problem; the role of the controller is to keep the system around the desirable steady state and reject disturbances that might occur because otherwise the production time would be disrupted, jeopardizing the feasibility of the schedule under execution. The optimal sequencing of tasks relies mostly on the transition times and so the control policy can have considerable impact on the schedule as the transition time is practically the time that the controller needs to take the system from one steady state to the next.

The simultaneous cyclic scheduling and dynamic optimisation of a single multi-product CSTR was studied by Flores-Tlacuahuac et al.[9]. The authors proposed a time-slot based formulations for the scheduling part of the problem, where equal number of slots and products were considered. Apart from model based strategies, the use of parametrised PI controllers[10] for the integration of cyclic scheduling and control has been proposed. Zhuge and Ierapetritou[11] proposed a framework for the closed loop implementation of the integrated solution of scheduling and control (iSC) for continuous processes that shared many similarities with model predictive control (MPC). The same authors, studied the iSC of batch processes through multi-parametric programming; they designed the multi-parametric controller offline and embedded the explicit solutions with additional constraints in the scheduling model[12]. In general, the iSC is formulated as a mixed integer dynamic optimisation problem (MIDO) and then following an numerical integration scheme is discretised into large scale mixed integer nonlinear programming problem (MINLP) which can be computationally demanding. To ease the computational burden for the case of iSC of a single multi-product CSTR the use of Benders decomposition has been proposed as an alternative solution technique[13]. The use of fast MPC in the context of iSC has also been reported, in which case linear piecewise affine approximations of the original nonlinear dynamics were employed[14]. One of the main challenges in the iSC stems from the different time scales involved in the two problems. Recently, "time-scale bridging" approaches have been proposed[15;16] where the main idea is to derive a low dimensional model for the dynamics of the system and thus create offline a correlation between system outputs and set-points in order to speed up the required calculations. More specifically, in Baldea et al.[17] a closed loop framework for the solution of the integrated cyclic scheduling and control was presented. The authors derived the corresponding time scale bridging model (SBM) and included it in the scheduling formulation as a set of soft constraints, while a scheduling-oriented MPC was designed for the closed loop implementation of the integrated solution. For further discussion the interested reader is referred to some recent reviews on the topic of iSC[3;8;18].

Recently, the development of frameworks for integrated planning, scheduling and control (iPSC) has started to receive attention. Prompted by the potential economic benefits that the iSC has indicated, the investigation of an even more integrated decision making framework that takes full advantage of all the possible interactions involved in the three problems constitutes a promising direction. Within the iPSC framework, the decisions involved in planning, scheduling and control are made simultaneously with a common objective. It can be understood that iPSC poses many challenges despite the potential benefits; the time-scale problem is further exacerbated when planning decisions are considered, the way that the three different problems are effectively linked constitutes another major factor that affects model complexity. The iPSC of single unit continuous manufacturing processes, for short term planning periods, was studied and formulated as an MINLP by Gutierrez-Limon et al.[19]. The authors employed the scheduling and planning model of Dogan and Grossmann[20] while for the control part of the iPSC a nonlinear MPC (NMPC) scheme was used. Following this work, the transition times are fixed offline based on heuristics and thus are not considered as decision variables. Note that despite the use of a NMPC scheme in the aforementioned work, disturbance rejection was not considered. The same authors[5] later on proposed a reactive heuristic strategy for the iPSC under the presence of unforeseen events. Shi et al.[21] considered the integration of planning, scheduling and dynamic optimisation of continuous manufacturing processes. The authors, proposed a technique to create a flexible-recipe framework in which pairs of transition times and cost are determined offline. In order to alleviate the computational complexity, they decomposed the problem, thus rendering it into a mixed integer linear programming (MILP) problem, for which a bi-level decomposition solution procedure was also proposed. Note that in their work, no disturbances are considered and the dynamic optimisation provides only open-loop related information about the real dynamics of the process. Again the model of Dogan and Grossmann[20] was used as a basis for the integrated planning and scheduling and the authors proposed an alternative way to calculate the inventory balance in every production period, based on the trapezoid rule.

1.2 Motivation and problem statement

The objective of the present article is to provide a computationally efficient framework for the integration of planning, scheduling and optimal control for the deterministic case where no uncertainty is considered at any of the levels of planning, scheduling and control. Motivated by the ever lasting need for more efficient and reliable operations in the process industries we aim to explore the interdependence of the decisions between the three different hierarchical levels which up until recently were considered in a decoupled manner. In general, we consider single unit continuous manufacturing processes which based on multiple steady states, that the underlying dynamic system exhibits, can produce a number of different products.

Concisely, the iPSC problem can be stated as follows:

Given:

- A single stage, multi-product continuous manufacturing process
- Production planning horizon
- Demands for each product at the end of each planning period
- Process dynamics and steady state operating conditions of the process
- Raw material, operating and inventory costs
- Selling prices

Determine:

- Dedicated production time and cost for each product in every planning period
- Optimal production sequences
- Optimal change-over times and cost
- Inventory and backlog level for each product at the end of each period
- Optimal dynamic trajectories of the process

Objective:

Maximise the production profit of the process; i.e. the revenue, minus inventory, backlog, operation, production and transition costs under deterministic assumptions. Note, that since in the present work no disturbances are considered at the level of dynamics, the optimal control part of the integrated problem is concerned with open-loop policies and thus we restrict ourselves to open-loop stable systems and the term optimal control is used in a dynamic optimisation sense.

Since the iPSC involves the optimal control of the process the problem is formulated as an MIDO which is discretised into an MINLP. The degrees of freedom for the optimisation within the iPSC involve among others: (i) production amounts within each planning period, (ii) assignment of products, (iii) transition times for the changeovers between products, (iv) optimal dynamic trajectories and (v) backlog of unmet demand. The remainder of the article is organised as follows: in section 2 the main parts of the methodology developed for the integrated problem are described. Next, in section 3 the proposed methodology is illustrated and compared through three different case studies with the time-slot based formulation for the integrated problem highlighting the computational savings achieved. Finally, in section 4 concluding remarks and future research directions are drawn.

2 Methodology

The majority of research work conducted for the integration of control with operations has focused on time-slot based formulations. In the present work, we propose a Travelling Salesman Problem (TSP) based framework for the integrated planning and scheduling problem that has two distinct features. First, the time representation used herein is hybrid, i.e. the planning periods are modelled as discrete time points while within each planning period a continuous time representation is followed. Secondly, following the proposed TSP formulation the notion of time-slots is replaced by implicitly unique pairs of products which can be produced in a sequential manner within each planning period.

2.1 Objective of the iPSC

As discussed in the previous section, the main reason that the iPSC is formulated in a simultaneous and not sequential manner is to take advantage of the information available across the different decision levels. Another reason and key objective of the present study is to provide a way of reflecting the process dynamics into process economics. The objective function of the integrated problem is the maximisation of profit and is calculated as the revenue minus the costs associated with the inventory, raw material consumption, backlogged demand and operation.

Eq.(1) represents the revenue (Φ_1) of the production as the summation of the sales of every product i, for every customer c, for every planning period ($\mathrm{S_{cip}}$) multiplied by its respective selling price ($\mathrm{P_i}$).

$$\Phi_1 = \sum_{\mathrm{c}} \sum_{\mathrm{i}} \sum_{\mathrm{p}} \mathrm{P_i S_{cip}} \tag{1}$$

Eq.(2) accounts for the total operational cost (Φ_2) over the planning horizon which is calculated as the product of the unitary operational cost ($\mathrm{C_i^{oper}}$) and the amount produced ($\mathrm{Pr_{ip}}$).

$$\Phi_2 = \sum_i \sum_p \mathrm{C_i^{oper} Pr_{ip}} \tag{2}$$

The total inventory cost is given by eq.(3) and is calculated as the product of the unitary inventory cost ($\mathrm{C_i^{inv}}$) and the inventory level ($\mathrm{V_{ip}}$) of product i at the end of every planning period p.

$$\Phi_3 = \sum_i \sum_p \mathrm{C_i^{inv} V_{ip}} \tag{3}$$

When demand cannot be met, in the present work backlog is allowed under a penalty. The cost associated with backlogged demand is calculated by eq.(4).

$$\Phi_4 = \sum_c \sum_i \sum_p \mathrm{CB_{ic} B_{cip}} \tag{4}$$

where $\mathrm{CB_{ic}}$ stands for the unitary backlog cost and $\mathrm{B_{cip}}$ denotes the demand of customer c at the end of planning period p for product i that is backlogged.

Another way planning, scheduling and optimal control interact is the calculation of the changeover cost. In principle, the changeover cost is calculated as the product of a unitary changeover cost by the binary variable that indicates the changeover occurrence. However, following the holistic approach that the iPSC dictates, the changeover cost is practically the utilisation of resources for the achievement of the next steady state, which from a control perspective is translated into the values of the control input during the transition period. Apart from that, the changeover costs account for any off-spec products that are manufactured during the transient period. In Figure 2, a conceptual graph for an arbitrary schedule is given.

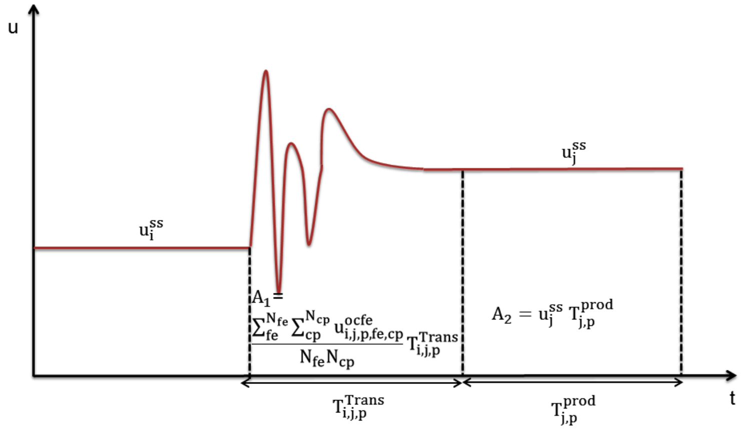


Figure 2: Calculation of raw material cost

As shown in Figure 2, the calculation of the raw material consumption cost during transition periods is computed as the integral of the arbitrary curve. The corresponding cost is numerically calculated following Radau IV quadrature as shown by eq. (5).

$$A_1 = \sum_m \sum_i \sum_j \sum_p \sum_{fe} \sum_{cp} u_{mijpfecp}^{ocfe} \cdot T_{ijp}^{Trans} \cdot h^{ocfe} \cdot \Omega_{cpN_{cp}} \tag{5}$$

The calculation of raw material consumption cost during the production of a product is simply calculated as the area of the rectangle defined by the production time (T_{ip}) and the pre-specified steady state value of the control input (u_{mi}^{ss}). For that reason the aforementioned cost is calculated as shown by eq. (6).

$$A_2 = \sum_m \sum_i \sum_p C_m^{raw} u_{mi}^{ss} T_{ip} \tag{6}$$

Overall the objective function to be maximised is the profit of the process which is given by eq. 7.

$$\text{PROF} = \Phi_1 - \Phi_2 - \Phi_3 - \Phi_4 - A_1 - A_2 \tag{7}$$

2.2 Modelling the planning and scheduling problem

For the integration of planning and scheduling in the present work a TSP model is employed. The model was originally proposed by Liu et al.[22] and proved to have computational benefits in comparison with the time-slot based formulation. Similar to the classic TSP problem where binary variables indicate the path from one city to another, the changeovers between two different products are modelled in a similar fashion. Following this model, the planning horizon is divided in typically equal-length planning periods which are modelled as discrete time points and within each planning horizon continuous time representation is employed for the detailed schedule. Next we present the equations that formulate the model. A visual representation of the hybrid time formulation involved in the TSP model is given in Figure 3.

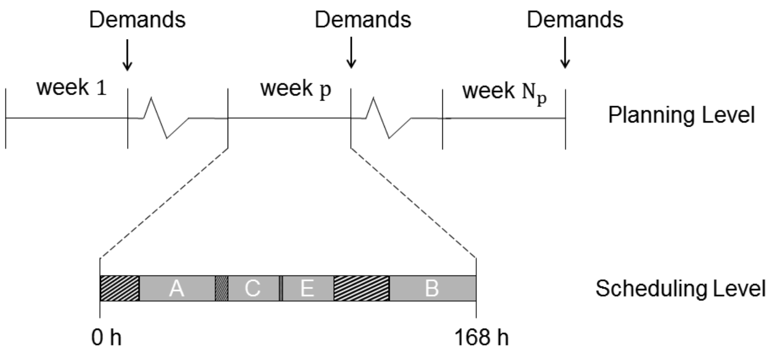


Figure 3: Hybrid time representation of the TSP model for the levels of planning and scheduling

As shown in Figure 3, demands for each product are satisfied at the end of each planning period and the inventory and backlog levels are calculated at those time points too. Within each time point (planning period), continuous time representation of total duration $\theta_{\mathrm{p}}^{\mathrm{up}}$ is employed for the modelling of decisions on a scheduling level. Notice that, a changeover between two adjacent periods, e.g. week p-1 and week p, occurs at the beginning of planning period p. In Figure 3, the blocks with the stripes are used to denote changeovers while the rest denote production of a product.

2.2.1 Allocation constraints

Only one product can be processed first in every planning period. To model this, the binary variable F_{ip} is introduced in eq.(8), which if equal to 1 indicates that product i is the first one to be produced in planning period p and zero otherwise.

$$\sum_{i}^{N} F_{ip} = 1 \qquad \forall p \tag{8}$$

where i is the index of products, N is the total number of products and p is the planning period. Eq.(9) ensures that only one product can be processed last in every planning period.

$$\sum_{i}^{N} L_{ip} = 1 \qquad \forall p \tag{9}$$

Similar to eq. (8) the binary variable L_{ip} is used to indicate whether or not product i is the last one to be processed in planning period p. Eq.(10) dictates that a product can be processed first only if it has been assigned to the planning period.

$$F_{ip} \leq E_{ip} \qquad \forall i,\ p \tag{10}$$

where E_{ip} is a binary variable that indicates whether product i is assigned for production in planning period p. To ensure that a product can be processed last, only if it has been assigned to the planning period, eq.(11) is used.

$$L_{ip} \leq E_{ip} \qquad \forall i,\ p \tag{11}$$

Notice, that the binary variables F_{ip} and L_{ip} are indicative of the sequence of tasks performed within each planning period as the order of the rest of tasks is computed implicitly by the changeovers.

2.2.2 Sequencing constraints

When moving from the production of a product i to another product j, a changeover occurs. To model changeovers within the same planning period the binary variable Z_{ijp} is used if product i precedes product j in planning period p.

$$\sum_{i \neq j}^{N} Z_{ijp} = E_{jp} - F_{jp} \qquad \forall j, p \tag{12}$$

Eq. (12) denotes that a product if assigned to a planning period, unless the first to be processed, results in a changeover with another assigned product. Next through eq.(13) it is ensured that a product unless the last to be processed, if assigned to the planning period, results in a changeover with another assigned product.

$$\sum_{j \neq i}^{N} Z_{ijp} = E_{ip} - L_{ip} \qquad \forall i, p \tag{13}$$

Finally, to model changeovers across adjacent weeks eq.(14)-(15) are used.

$$\sum_{i}^{N} Zf_{ijp} = F_{jp} \qquad \forall j, p > 1 \tag{14}$$

$$\sum_{j}^{N} Zf_{ijp} = L_{i,p-1} \qquad \forall i, p > 1 \tag{15}$$

where the binary variable Zf_{ijp} is used to model changeovers between adjacent planning periods.

2.2.3 Symmetry breaking constraints

In order to avoid the enumeration of symmetric solutions and exclude infeasible production sub-cycles the integer variable O_{ip} (order index) is introduced and denotes the order at which the product i is processed during planning period p. Eq. (16)-(18) ensure the exclusion of such subcycles.

$$O_{jp} - (O_{ip} + 1) \geq -M(1 - Z_{ijp}) \qquad \forall i, j \in I,\ j \neq i,\ p \tag{16}$$

$$O_{ip} \leq M \cdot E_{ip} \qquad \forall i, p \tag{17}$$

$$\mathrm{F_{ip}} \leq \mathrm{O_{ip}} \leq \sum_{\mathrm{i}}^{\mathrm{N}} \mathrm{E_{ip}} \qquad \forall \mathrm{i}, \mathrm{p} \tag{18}$$

2.2.4 Timing constraints

At the core of the proposed model is the hybrid time formulation. Production ($\mathrm{T_{ip}}$) and transition time ($\mathrm{T^{trans}_{ijp}}$) are modelled in a continuous way. Lower and upper bounds on processing time are imposed through eq.(19).

$$\theta^{\mathrm{lo}}_{\mathrm{p}} \mathrm{E_{ip}} \leq \mathrm{T_{ip}} \leq \theta^{\mathrm{up}}_{\mathrm{p}} \mathrm{E_{ip}} \qquad \forall \mathrm{i}, \mathrm{p} \tag{19}$$

where $\theta^{\mathrm{lo}}_{\mathrm{p}}$, $\theta^{\mathrm{up}}_{\mathrm{p}}$ constitute lower and upper bounds respectively. The changeover time across two adjacent periods can be split into two parts in different time periods based on eq.(20) which is adopted from the work of Kopanos et al.[23].

$$\mathrm{CT1_p} + \mathrm{CT2_{p-1}} = \sum_{\mathrm{i}} \sum_{\mathrm{j}} \mathrm{T^{trans}_{ijp}} \cdot \mathrm{Zf_{ijp}} \qquad \forall \mathrm{p} > 1 \tag{20}$$

The time balance within each planning period is then given by eq.(21).

$$\sum_{\mathrm{i}}^{\mathrm{N}} \mathrm{T_{ip}} + \sum_{\mathrm{i}}^{\mathrm{N}} \sum_{\mathrm{j} \neq \mathrm{i}}^{\mathrm{N}} (\mathrm{Z_{ijp}} \cdot \mathrm{T^{trans}_{ijp}}) + \mathrm{CT1_{p_{|p>1}}} + \mathrm{CT2_{p_{|p<|P|}}} \leq \theta^{\mathrm{up}}_{\mathrm{p}} \qquad \forall \mathrm{p} \tag{21}$$

Note that the eq.(19)-(21) allows for idle production time during the planning periods that the plant needs not to be utilised at its full production capacity. Even though, in the present work we consider planning periods of one week, i.e. 168h, the parameter $\theta^{\mathrm{up}}_{\mathrm{p}}$ can be modified to facilitate varying planning periods.

2.2.5 Production constraints

The amount of product i produced within period p ($\mathrm{Pr_{ip}}$) is calculated based on eq. (22) as the dedicated production time within that period ($\mathrm{T_{ip}}$) and the associated production rate ($\mathrm{r_i}$).

$$\mathrm{Pr_{ip} = r_i T_{ip} \qquad \forall i, p} \tag{22}$$

Eq.(23) is used for the calculation of the backlog ($\mathrm{B_{cip}}$) for the demand from customer c at the end of the current planning period, as the amount of backlog at the previous planning period ($\mathrm{B_{ci,p-1}}$) plus the demand ($\mathrm{D_{cip}}$) of the current planning period minus the related sales ($\mathrm{S_{cip}}$).

$$\mathrm{B_{cip} = B_{ci,p-1} + D_{cip} - S_{cip} \qquad \forall c, i, p} \tag{23}$$

The level of inventory ($\mathrm{V_{ip}}$) of product i at the end of planning period p, is related to the amount produced and the sales for that product through eq. (24).

$$\mathrm{V_{ip} = V_{i,p-1} + Pr_{ip} - \sum_c S_{cip} \qquad \forall i, p} \tag{24}$$

In addition to eq. (24), eq. (25) may be included in the iPSC formulation so as to model capacity considerations in terms of minimum ($\mathrm{V_i^{min}}$) and maximum ($\mathrm{V_i^{max}}$) allowable inventory levels.

$$\mathrm{V_i^{min} \leq V_{ip} \leq V_i^{max} \qquad \forall i, p} \tag{25}$$

2.3 Dynamic optimisation (DO)

In this section, we present the mathematical formulation used for the dynamic optimisation/ optimal control of the process. Consider the following generic continuous dynamic system which can be either linear or nonlinear and is given by eq. (26)-(27).

$$\mathrm{\frac{dx}{dt} = f(x(t), u(t)) \quad x_0 = x(t|_{t=0})} \tag{26}$$

$$\mathrm{y(t) = h(x(t), u(t))} \tag{27}$$

where $x(t) \in X \subseteq R^{n_x}$, denotes the time-variant vector of state variables, $u(t) \in U \subseteq R^{n_u}$, denotes the time dependent control input vector and $y(t) \in Y \subseteq R^{n_y}$ denotes the time dependent output vector. Note that X, Y and Z correspond to their respective admissible set. $f : \mathbb{R}^{n_x+n_u} \rightarrow \mathbb{R}^n$ is a C^2 vector field and $h : \mathbb{R}^{n_x+n_y} \rightarrow \mathbb{R}^{n_y}$ can be an either linear or nonlinear map. In order to transform the dynamic system into an algebraic one, a discretisation scheme has to be employed. This can be done either explicitly by integrating numerically eq. (26)-(27), considering them as boundary value problem (BVP) through direct single or multiple shooting methods or implicitly following a simultaneous scheme. For the case that constraints need to be considered the sequential methods are not appropriate as they cannot facilitate such requirement easily[24].

In the present work, orthogonal collocation on finite elements (OCFE) was chosen for the discretisation of the dynamic problem because of its desirable properties in terms of numerical stability[25;26]. OCFE belongs to the family of simultaneous approaches and is also known as direct transcription method. Following OCFE, both the control and the state variables are discretised in time. The domain of time is discretised into a number of finite elements and within each finite element a number of collocation points is considered. The DO problem is transformed into an nonlinear programming (NLP) problem by approximating the control and state profiles, across the finite elements, with a family of orthogonal polynomials such as Lagrange or Legendre polynomials. A thorough discussion on simultaneous solution strategies for dynamic optimisation is conducted in Biegler[24].

Because of the integrated nature of the problem the state and control variables have to be tracked in every collocation point (cp) of every finite element (fe) of every unique sequence $i \rightarrow j$ in every planning period (p) and they are denoted as $x^{ocfe}_{nijpfecp}$ and $u^{ocfe}_{mijpfecp}$ respectively. The continuous time is discretised through eq. (28)

$$\tilde{t}_{ijpfecp} = ((fe - 1) + roots_{cp})\frac{T^{trans}_{ijp}}{N_{fe}} \qquad \forall i, j, p, fe, cp \tag{28}$$

where $roots_{cp}$ are the roots of the orthogonal polynomial used within the OCFE and N_{fe} is the cardinality of the set of finite elements. Eq.(29) is employed for the numerical solution of the ODE using OCFE.

$$\dot{x}_{nijpfecp} = f^{n}(x^{ocfe}_{nijpfecp},\ u^{ocfe}_{mijpfecp},\ \sigma), \qquad \forall n, m, i, j, p, fe, cp \tag{29}$$

Eq.(29) is used for the computation of the numerical value of the derivative of the n^{th} state based on the associated differential equation that governs the related state. Note, that the right hand side of eq.(29) denotes is the discretised equivalent from the ODE related to the n^{th} state.Continuity of the state variables across adjacent finite elements is imposed by eq.(30)

$$x^{ocfe_{init}}_{nijpfe} = x^{ocfe_{init}}_{nijp,fe-1} + T^{trans}_{ijp} \cdot h^{ocfe} \sum_{cp=1}^{n_{cp}} \Omega_{cpN_{cp}} \dot{x}_{nijp,fe-1,cp} \qquad \forall n, i, j, fe > 1 \tag{30}$$

The numerical solution of the state profiles across the discretised domain is computed by eq.(31)

$$x^{ocfe}_{nijpfecp} = x^{ocfe_{init}}_{nijpfe} + T^{trans}_{ijp} \cdot h^{ocfe} \sum_{cpp=1}^{n_{cp}} \Omega_{cpp\,cp} \dot{x}_{nijpfecpp} \qquad \forall n, i, j, fe, cp \tag{31}$$

Note that in general, variable steps (h^{ocfe}) and continuity constraints on the profiles of the control variables may be employed, if required for the problem under study; however in the present work we do not account for such cases.

2.4 Linking variables between DO, scheduling and planning model

Tracking the dynamic trajectory of the system can be translated into a regime of production. In the context of iPSC, changeovers can be defined as the time needed by the system to move from one steady state to the next one. Similarly, the production time can be defined as the time that the system is stabilised around the desirable steady state in order to manufacture a certain amount of products that would satisfy the demand. Ideally, one would have to perform a discretisation of the dynamics across the entire dynamic trajectory but in the present work since no process disturbances are considered we assume that once the steady state is achieved the system remains in steady state unless a changeover occurs. Therefore, the discretisation of the dynamics is employed only for the transient periods of changeovers. In general, the linking between the DO and the scheduling and planning model is achieved with eq. (32)-(35).

$$\mathrm{x}^{\mathrm{in}}_{\mathrm{nijp}} = \mathrm{x}^{\mathrm{ocfe_{init}}}_{\mathrm{nijpfe}} \qquad \forall \mathrm{n}, \mathrm{i}, \mathrm{j}, \ \mathrm{i} \neq \mathrm{j}, \ \mathrm{fe} = 1 \tag{32}$$

$$\mathrm{u}^{\mathrm{in}}_{\mathrm{mijp}} = \mathrm{u}^{\mathrm{ocfe}}_{\mathrm{mijpfecp}} \qquad \forall \mathrm{m}, \mathrm{i}, \mathrm{j}, \ \mathrm{i} \neq \mathrm{j}, \ \mathrm{fe} = 1, \mathrm{cp} = 1 \tag{33}$$

$$\mathrm{x}^{\mathrm{fin}}_{\mathrm{nijp}} = \mathrm{x}^{\mathrm{ocfe}}_{\mathrm{nijpN_{fe}N_{cp}}} \qquad \forall \mathrm{n}, \mathrm{i}, \mathrm{j}, \ \mathrm{i} \neq \mathrm{j} \tag{34}$$

$$\mathrm{u}^{\mathrm{fin}}_{\mathrm{mijp}} = \mathrm{u}^{\mathrm{ocfe}}_{\mathrm{mijpN_{fe}N_{cp}}} \qquad \forall \mathrm{m}, \mathrm{i}, \mathrm{j}, \ \mathrm{i} \neq \mathrm{j} \tag{35}$$

The new variables introduced here are $\mathrm{x}^{\mathrm{in}}_{\mathrm{nijp}}$, $\mathrm{u}^{\mathrm{in}}_{\mathrm{mijp}}$, $\mathrm{x}^{\mathrm{fin}}_{\mathrm{nijp}}$ and $\mathrm{u}^{\mathrm{fin}}_{\mathrm{mijp}}$. The first two variables define the value of the state and control inputs at the beginning of the transition and the last two are used in a similar fashion for the end of the transition. Eq. (32) ensures that the value of the discretised state variable ($\mathrm{x}^{\mathrm{ocfe_{init}}}_{\mathrm{nijpfe}}$) at the *beginning* of the first finite element is equal to the initial condition of the system at the beginning of the transition, while eq. (33) is employed for the control input. At the *end* of the transition the state of the system must have reached a certain value ($\mathrm{x}^{\mathrm{fin}}_{\mathrm{nijp}}$) and eq. (34) imposes that value of the discretised state variable at the last collocation point ($\mathrm{N_{cp}}$) of the last finite element ($\mathrm{N_{fe}}$) is such that the transition terminates. Finally, eq. (35) has similar functionality with eq. (34) but for the discretised control input. A conceptual graph about the linking between DO and scheduling is given in Figure 4.

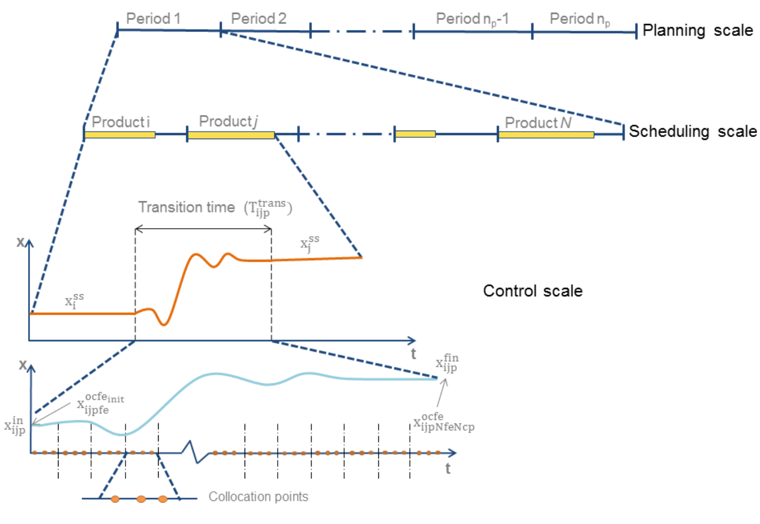


Figure 4: Associating the dynamics during an arbitrary transition from product i to product j

In Figure 4, the multi-scale nature of the problem is illustrated. On the top graph, the planning scale is modelled as discrete time points each of which is then expanded in a continuous time domain for the scheduling scale. The scheduling scale is then further analysed into the control scale and it is shown how the process moves from the production of product i to product j. At the beginning, the system is regulated around the steady state of product i until a changeover occurs in which case a transition from the steady state of product i (x^{ss}_{ni}) to the steady state of the next product, e.g. j, (x^{ss}_{nj}) is initiated. On the bottom graph, the dynamics of the system throughout this transition are envisaged. Note, that the system at the beginning of the transition starts from (x^{ss}_{ni}) and thus the discretised state variable of the first finite element, i.e. $x^{ocfe_{init}}_{nijpfe|_{fe=1}}$, must be equal to that value. During the dynamic optimisation, the time is discretised in finite elements (intervals between consecutive blue dashed lines in Figure 4) and within each finite element a certain number of collocation points are defined (orange dots).

2.5 Linking equations between DO and TSP planning and scheduling

Now that the linking variables between DO and scheduling have been established, it remains to provide the physical meaning of these variables in terms of production scheduling. Since, x^{in}_{nijp} and x^{fin}_{nijp}, correspond to the initial and final values of the transitions between different products it follows that they are also associated with the steady state operation of the system when production takes place. Indeed, the initial value of the state variables at the beginning of a transition should be equal to the steady state of the product that was being processed before the changeover occurred. Similarly, since the transition between two products is terminated once the system has reached the next steady state, the final value of the state variables at the end of the transition must be equal to the steady state of the following product. The same holds for the control variables.

Since in the present work a TSP based planning and scheduling model is adapted, in contrast with the time-slot based formulations, the binary variable that can be used to express mathematically the aforementioned conditions is the Z_{ijp} for transitions that occur within the same planning period and

$\mathrm{Zf_{ijp}}$ for transitions between adjacent planning periods. The final set of constraints that constitute the iPSC model are given by eq. (36)-(43).

$$\mathrm{x^{in}_{nijp} = x^{ss}_{ni} \cdot Z_{ijp} \qquad \forall n, i, j,\ i \neq j,\ p = 1} \tag{36}$$

$$\mathrm{u^{in}_{mijp} = u^{ss}_{mi} \cdot Z_{ijp} \qquad \forall m, i, j,\ i \neq j,\ p = 1} \tag{37}$$

$$\mathrm{x^{in}_{nijp} = x^{ss}_{ni} \cdot (Z_{ijp} + Zf_{ijp}) \qquad \forall n, i, j,\ i \neq j,\ p > 1} \tag{38}$$

$$\mathrm{u^{in}_{mijp} = u^{ss}_{mi} \cdot (Z_{ijp} + Zf_{ijp}) \qquad \forall m, i, j,\ i \neq j,\ p > 1} \tag{39}$$

$$\mathrm{x^{fin}_{nijp} = x^{ss}_{nj} \cdot Z_{ijp},\ \forall n, i, j,\ i \neq j,\ p = 1} \tag{40}$$

$$\mathrm{u^{fin}_{mijp} = u^{ss}_{mj} \cdot Z_{ijp} \qquad \forall m, i, j,\ i \neq j,\ p = 1} \tag{41}$$

$$\mathrm{x^{fin}_{nijp} = x^{ss}_{nj} \cdot (Z_{ijp} + Zf_{ijp}) \qquad \forall n, i, j,\ i \neq j,\ p > 1} \tag{42}$$

$$\mathrm{u^{fin}_{mijp} = u^{ss}_{mj} \cdot (Z_{ijp} + Zf_{ijp}) \qquad \forall m, i, j,\ i \neq j,\ p > 1} \tag{43}$$

Eq.(36)-(37) impose that the initial values of the state and control variables respectively are equal to the steady state values of product i, which is the precedent product in the changeover for the first planning period. After the first planning period a changeover might occur at the beginning of this period, in which case the binary variable $\mathrm{Zf_{ijp}}$ is activated, to indicate this transition from the previous week to the current one. Because of that, in eq. (38)-(39) we include the summation of the two changeover binary variables, i.e. $\mathrm{Z_{ijp}}$, $\mathrm{Zf_{ijp}}$.

2.6 Monolithic and decomposed integration of planning, scheduling and optimal control

2.6.1 Monolithic iPSC

Integrating the decision levels of planning, scheduling and optimal control for continuous manufacturing processes results in an MIDO problem, where the decisions are made simultaneously across all three levels under a common objective, the maximisation of profit. As presented in the previous sections, in the present work we employ the model of Liu et al.[22] for the problem of simultaneous planning and scheduling and then OCFE is used for the discretisation of the dynamics of the system for the optimal control. The optimal control is linked using the constraints and auxiliary variables presented in section 2.5. Overall, the monolithic model for the iPSC consists of the following:

$$\begin{aligned}
\textbf{Monolithic iPSC}: \quad \max \quad \mathrm{PROF} = \quad & \Phi_1 - \Phi_2 - \Phi_3 - \Phi_4 - \mathrm{A}_1 - \mathrm{A}_2 \\
\text{Subject to}: \quad \text{eq.}(8) - (25) \quad & (\text{TSP Planning} - \text{Scheduling}) \\
\text{eq.}(28) - (31) \quad & (\text{Dynamic Optimisation}) \\
\text{eq.}(32) - (43) \quad & (\text{Linking constraints})
\end{aligned}$$

2.6.2 Decomposed iPSC

To alleviate the computational burden associated with the monolithic formulation of the iPSC, in the present work we propose a decomposition of the problem through the solution of offline DOs and the development of linear metamodels to associate the transition time with transition cost. The decomposition is based on the grounds of the following two observations:

1. Formulating and solving the monolithic iPSC results typically in large scale non-convex MINLPs problems which are difficult to solve and the use of global optimisation solvers is rather difficult due to the scale of the MINLPs [21;27]. Within the manufacture, being in a position to provide on time good solutions is crucial and with the monolithic MINLPs such requirement may not be always satisfied. Upon inspection, apart from the time-scale problem that is inherent to the iPSC, the solution of the underlying dynamic optimisation problem constitutes the main bottleneck because of the consideration of the transition times as decision variables. In the literature, ways for dealing with this problem include, fixing the transition time matrix in an offline step based on heuristics [19] or creating pre-computed recipes that include couples of transition time and cost [21]. The disadvantage of following the aforementioned alternatives are for the first one that it does not reflect a true integration among the levels of iPSC and the latter assumes that the decision maker will always face one of the pre-specified realisations of transition time and cost.

2. To the best of the authors' knowledge, in none of the research works conducted for the iPSC of continuous processes the effect of disturbance at control level has been accounted for. In order to compensate for the effect of disturbances, one would have to employ a feedback control mechanism. To this effect, once a disturbance is realised, the decision maker would possibly need to re-schedule. It can be understood then, that the monolithic iPSC would have to be solved repeatedly, in decreased decision space (as some of the decisions would have already been fixed), but at a fast computational time. This cannot be done given the scale and nonconvexity of the problem as will be illustrated later on by the case studies, given the current computational power at hand. It follows that the feedback mechanism / closed-loop control should be considered in an outer loop rather than within the iPSC formulation.

In Figure S1, the flow of information across the different levels of decision making can be envisaged. As shown, the main information shared between the level of optimal control and scheduling is the transition times and the transition cost. Of course, the dynamics of the system given a certain transition time can be determined for the open loop "control" case, which is the one of interest of this work. In order to exploit this interaction, in the literature, a method of creating pre-computed pairs of transition time and cost has been proposed[21]. The drawbacks of following such an approach is the increase in the number of binary variables introduced in the iPSC model formulation for the selection of the specific pair of transition time-cost as well as it does not necessarily treat the case where a feedback controller is used and a realisation of the system's dynamics other than the pre-computed ones is observed. To this effect, linear metamodels are developed so as to carry the aforementioned information between the levels of optimal control and scheduling. The reason for that is two-fold: (1) through the use of the metamodels the transition times are still allowed to be continuous decision variables of the integrated problem, allowing for instances where the closed loop behaviour differs from the open loop thus resulting in different transition times than the minimum ones and (2) the procedure of building the linear metamodels is carried out offline and the problems associated are NLPs of moderate size for which global optimisation solvers can possibly be employed. As will be shown in the next section, through the case studies examined, the law that correlates transition time and transition cost is of logarithmic nature for large time scales but for shorter ones it can be approximated precisely by the linear metamodels. As far as the dynamic open-loop trajectories are concerned, with the transition time fixed the control and state variables can be calculated through the solution of the related optimal control problem in a subsequent step. However, for the deterministic case which is under study in the present work the decomposed model will always choose the minimum transition times because it infers minimum cost and so that particular dynamic trajectory is stored and employed.

For the decomposed framework of the iPSC (decomposed iPSC for short), first the minimum transition times for any possible transition are computed based on problem (Offline DO part I).

$$\textbf{Offline DO part I}: \quad \tau_{\mathrm{ij}}^{\mathrm{min}} = \min_{\mathbf{x}^{\mathrm{ocfe}},\ \mathbf{u}^{\mathrm{ocfe}}} \quad \mathrm{T}_{\mathrm{ij}}^{\mathrm{trans}}$$

$$\text{Subject to}: \quad \text{eq.}(28) - (31) \quad \text{(Dynamic Optimisation)}$$

$$\text{eq.}(32) - (43) \quad \text{(Linking constraints)}$$

Offline DO part I, is a non-convex NLP even for the case that linear dynamics govern the production system, since within the numerical integration, the time is considered as the objective variable. After the transition time is computed for each possible product combination, the procedure of building the linear metamodels follows. In the present work, the transition time is allowed to vary up to 3 times the minimum transition time. Problem (Offline DO part II), is again an NLP and creates the data samples that will be used for the linear metamodels.

$$\textbf{Offline DO part II}: \quad \min_{\mathbf{x}^{\mathrm{ocfe}},\ \mathbf{u}^{\mathrm{ocfe}}} \quad \mathrm{CT}_{\mathrm{ij}}^{\mathrm{tran}}$$

$$\text{Subject to}: \quad \text{eq.}(28) - (31) \quad \text{(Dynamic Optimisation)}$$

$$\mathrm{T}_{\mathrm{ij}}^{\mathrm{trans}} \in [\tau_{\mathrm{ij}}^{\mathrm{min}},\ 3\tau_{\mathrm{ij}}^{\mathrm{min}}] \quad \text{(Variable transition time)}$$

In order to create a sufficient number of data points, a sampling method needs to be followed. After choosing the number of points ($\mathrm{n_{sample}}$) the following computational routine (Meta_sample) is performed.

Meta_sample:

$T_{ij}^{trans} = \tau_{ij}^{min}$

While iter $\leq n_{sample}$:

$$T_{ij}^{trans} = T_{ij}^{trans} + \tau_{ij}^{min} \cdot \frac{t^{max}}{n_{sample}}$$

Solve (Offline DO part II)

$$iter = iter + 1$$

where t^{max} denotes the maximum variance from the minimum transition time allowed, e.g. in the present work $t^{max} = 2$.

The output of this computational step, which is performed offline, is a set of points correlating transition time and cost for each transition. With the sample data computed, the next step is to create the metamodels. In the present work, the Statsmodels 0.6.1[28] module from Python was employed for the creation of the linear metamodels. A general form of the linear metamodels is given by eq. (44).

$$CT_{ij}^{tran} = \alpha_{ij} T_{ij}^{trans} + \beta_{ij} \qquad \forall i, j \in I, \; i \neq j \tag{44}$$

where α_{ij}, β_{ij} are $N \times N$ matrices, denoting the slope and intercept of the linear metamodel respectively. Once the metamodels and the minimum transition times are computed the next step is to form the final decomposed iPSC model. Ideally, the transition times should be kept as decision variables within the decomposed iPSC while allowing again the changeovers between two adjacent planning periods to be split. When the transition times are decision variables, bilinear terms of the form $T_{ijp}^{trans} \cdot Z_{ijp}$ or $T_{ijp}^{trans} \cdot Zf_{ijp}$ appear. Exact linearisation of such bilinear terms can be achieved based on the following[29]:

$$T_{ijp}^{trans_{lin_1}} \geq T_{ijp}^{trans} + (Z_{ijp} - 1) \cdot \tau_{max} \qquad \forall i, j \in I,\ i \neq j, p \tag{45}$$

$$T_{ijp}^{trans_{lin_2}} \geq T_{ijp}^{trans} + (Zf_{ijp} - 1) \cdot \tau_{max} \qquad \forall i, j \in I, p > 1 \tag{46}$$

$$T_{ijp}^{trans_{lin_1}} \leq T_{ijp}^{trans} \qquad \forall ij \in I,\ i \neq j, p \tag{47}$$

$$CT1_p + CT2_{p-1} = T_{ijp}^{trans_{lin_2}} \qquad \forall i, j \in I, p > 1 \tag{48}$$

$$T_{ijp}^{trans_{lin_2}} \leq T_{ijp}^{trans} \qquad \forall i, j \in I, p > 1 \tag{49}$$

In eq. (45)-(49), new variables are introduced, $T_{ijp}^{trans_{lin_1}}, T_{ijp}^{trans_{lin_2}}$, which are the linear counterparts of the aforementioned bilinear terms. Notice, that this is achieved either when Z_{ijp} or Zf_{ijp} is equal to 1, thus indicating the corresponding changeover between products. In addition to that, the transition time between products should be bounded from below based on eq.(50).

$$T_{ijp}^{trans} \geq \tau_{ij}^{min} \qquad \forall i, j \in I,\ i \neq j, p \tag{50}$$

The linear counterpart of the bilinear terms ($T_{ijp}^{trans} \cdot Z_{ijp}$ or $T_{ijp}^{trans} \cdot Zf_{ijp}$) is also used in the metamodels. The objective of the decomposed iPSC is the same as the one used in the monolithic formulation with the exception of the term A_1 which is substituted by eq. (51).

$$B_1 = \sum_p \sum_i \sum_{j \neq i} \alpha_{ij} (T_{ijp}^{Trans_{lin_1}} + T_{ijp_{|p>1}}^{Trans_{lin_2}}) + \beta_{ij} (Z_{ijp} + Zf_{ijp}) \tag{51}$$

Overall, the decomposed iPSC model is an MILP and is formulated as follows:

$$\textbf{Decomposed iPSC}: \quad \max \quad \mathrm{PROF} = \quad \Phi_1 - \Phi_2 - \Phi_3 - \Phi_4 - \mathrm{B}_1 - \mathrm{A}_2$$

$$\text{Subject to}: \quad \text{eq.}(8) - (25) \quad (\text{TSP Planning} - \text{Scheduling})$$

$$\text{eq.}(45) - (50) \quad (\text{Time linearisation})$$

3 Case Studies

A number of case studies are presented in the next section to demonstrate the advantages of the proposed modelling framework for the iPSC. The first one examines the iPSC of a single-input single-output (SISO) multi-product CSTR; the second one, a multiple-input multiple-output (MIMO) non-isothermal multi-product CSTR while the third one studies methyl methacrylate (MMA) polymerisation process. The pattern followed in this section is as follows: first, a comparison between the monolithic and decomposed iPSC models is given, for both the TSP and the time-slot based formulation, and then the decomposed approach is tested under different planning horizons, namely 4, 6 and 12 weeks.

All the optimisation problems, for the monolithic approach, are formulated as MINLPs and solved using GAMS 24.4.1[30] on a Dell workstation with 3.70 GHz processor, 16GB RAM and Windows 7 64-bit operating system. Finally, the optimisation problems corresponding to the decomposed approach are formulated as MILPs and modelled in GAMS 24.4.1 and solved using CPLEX 12.6.1.

Finally, for the comparison between the TSP and the time-slot based model for the iPSC some modifications need to be made with respect to the existence of idle time within the planning period, backlog of unmet demand and inventory calculation. The time-slot based model was proposed by Erdirik-Dogan and Grossmann[20] (E-D &G) and the corresponding model is given in Appendix A. As far as the inventory calculation is concerned the TSP model proposed by Liu et al.[22], considers inventory calculation on a weekly basis whereas E-D&G employ a linear overestimation of the inventory curve; to this effect, eq.(A.14)-(A.17) are replaced by eq.(24). Next, in E-D&G, the demand serves as lower bound to the level of sales at the end of each planning period and backlog is not considered; in order to account for backlog, eq.(A.18) is replaced by eq.(23). Finally, idle time is allowed between planning period by modifying eq.(A.11) as shown in eq.(52).

$$\mathrm{T^e_{N_sp}} + \sum_{\mathrm{i}}\sum_{\mathrm{j\neq i}} \tau_{\mathrm{ij}} \mathrm{Z'_{ijp}} \leq \mathrm{T^s_{1,p+1}} \qquad \forall \mathrm{p} = 1, \ldots, \mathrm{N_p} - 1 \tag{52}$$

3.1 SISO multi-product CSTR

First, the iPSC of a multi-product SISO CSTR that produces five different products, namely, A, B, C, D, E, based on the concentration and the volumetric flow of the reactant, is considered. The steady state operation points of the system are computed in an offline step. At the dynamic optimisation level, the state variable of the system is the concentration of the reactant ($\mathrm{C_R}$), while the control input is the volumetric flow of the liquid (Q). The reaction is 3^{rd} order irreversible, i.e. $R \xrightarrow{k} 3P$, $-\mathscr{R}_R = kC_R^3$. The nonlinear dynamic model of the system is given by:

$$\frac{\mathrm{dC_R}}{\mathrm{dt}} = \frac{\mathrm{Q}}{\mathrm{V}}(\mathrm{C_0} - \mathrm{C_R}) + \mathscr{R}_R \tag{53}$$

where $\mathrm{C_0}$ denotes the concentration of the reactant in the feed stream, V is the reactor volume and k is the reaction's kinetic constant. Assuming that, $\mathrm{V = 5000L}$, $\mathrm{C_0 = 1mol/L}$ and $k = 2\mathrm{L^2/mol^2h}$ the aim of the iPSC is to maximise the profit of the process while satisfying the demand as shown in Table 1.

Table 1: Demand and cost data for the SISO CSTR case study

	Planning Period		Operation cost ($/m^3)	Price ($/m^3)
Demand (m^3)	P_1	P_2		
A	400	0	0.13	200
B	3000	8000	0.22	150
C	7000	1200	0.35	130
D	15000	0	0.29	125
E	31000	20000	0.25	120

The system based on the given design parameters can exhibit multiple steady state at which different products can be produced. The rate of production for each product can be calculated as $r_i = Q_i^{ss} C_0 (\frac{C_0 - C_i^{ss}}{C_0})$. The related kinetic information are provided in Table 2.

Table 2: Kinetic data for the SISO CSTR case study

products	x_{ss}^i(mol/L)	u_{ss}^i(L/h)	r_i(mol/h)
A	0.0967	10	9.033
B	0.2000	100	80.000
C	0.3032	400	278.720
D	0.3930	1000	607.000
E	0.5000	2500	1250.000

Because of the order of the reaction the corresponding optimisation problem is formulated as an MINLP. Initially, we consider two planning periods, each one spanning a week (168h) and employ 20 finite elements with 3 collocation points for the discretisation of the corresponding dynamic system. Following the proposed framework, the minimum transition times and the linear metamodels are calculated offline. In Table 3, a comparison between the performance of BARON 14.4, CONOPT3 and ANTIGONE is provided. The computation of the minimum transition times results in the solution of 20 NLPs and Table 4 provides the related times.

Table 3: Problem statistics for the offline computation of the minimum transition time ($\tau_{\mathrm{i,j}}^{\mathrm{min}}$) for the SISO CSTR case study

Solver	CONOPT3	BARON	ANTIGONE
Type	NLP	NLP	NLP
Solution status	Locally optimal	Optimal	Optimal
Constraints	204	204	204
Cont. Var.	266	266	266
CPU (s)*	1.059	23,452	149.632

*Cumulative computational time for all the transitions

Table 4: Minimum transition times between products for the SISO CSTR case study

$\tau_{\mathrm{i,j}}^{\mathrm{min}}$ (h)	**A**	**B**	**C**	**D**	**E**
A	-	0.21	0.47	0.85	1.64
B	20.99	-	0.26	0.61	1.43
C	24.6	3.62	-	0.31	1.21
D	25.72	4.74	1.13	-	0.87
E	26.34	5.38	1.76	0.64	-

The linear metamodels are built next following the sampling technique described in section 2.6.2. While building the linear metamodels, the majority has a value of $\mathrm{R}^2 \geq 0.99$ but some fail to reach this desired threshold like the one shown in Figure 5 which corresponds to the transition from product C to product A. The total number of metamodels that have $\mathrm{R}^2 \leq 0.99$ are four out the twenty but for the sake of computational complexity we allow this approximation as it still reflects the impact that the dynamics of the system have in the production scheduling. Note that piecewise linear approximation could have been employed but that would lead in increase of the number of binary variables needed.

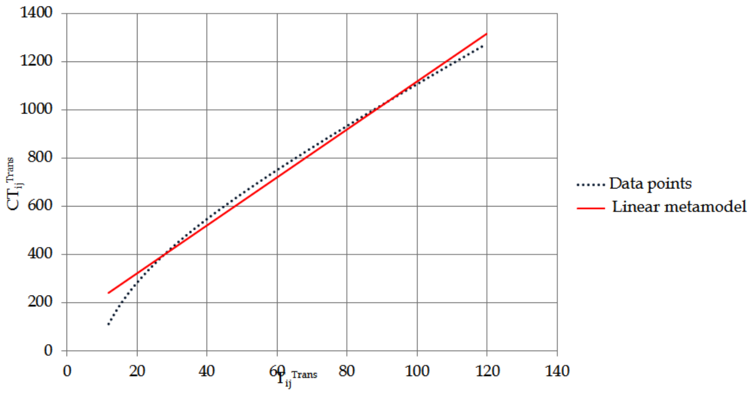


Figure 5: Graph of the linear metamodels built from sampling data for the transition from C to A

In general it was noticed based on the simulations that were conducted, that the law that governs the relation between transition time and cost is of logarithmic nature for large time scales; however, from a production scheduling perspective for the instance for the transition from C to A a delay of the transition of the order of hours would probably result in rescheduling thus the effect of offset from the metamodel can be circumvented. In any case, as mentioned in section 2.6.2, the aim of building the corresponding metamodels is to provide a computationally favorable correlation between the process dynamics and process economics within the context of iPSC. In Table S1, the corresponding coefficients of the slope and the intercept of the linear metamodels are given.

Once the metamodels are built, the monolithic and the decomposed integrated problems are formulated and solved in GAMS. Results for the SISO CSTR case study for planning horizon of 2 weeks are shown in Table 5.

Table 5: Results for the SISO CSTR case study for planning horizon of 2 weeks with no backlog and inventory constraints. OCFE with 20 finite elements and 20 collocation points was employed for the discretisation of the DO part

Model	Monolithic TSP	Monolithic T-S	Decomposed iPSC	
Type	MINLP		MILP (TSP)	MILP (T-S)
Constraints	8,557	3,170	287	581
Cont. Var.	10,841	3,551	256	488
Binary Var.	105	300	105	300
Solver	SBB/CONOPT3		CPLEX 12.6.1	
Profit ($)	8862971.18		9190688.58	
CPU (s)	274.780	995.539	0.078	3.5
Optimal	$P_1 : B \rightarrow C \rightarrow D \rightarrow A \rightarrow E$		P1: A→B→C→D→E	
Schedule	$P_2 : B \rightarrow C \rightarrow E$		P2: E→C→B	
$T^{trans}_{i,j,p}$(h)	P_1:0.575, 0.687 , 57.881, 3.680 P_2:12.104 , 0.575, 2.631		P_1: 0.211, 0.256 , 0.305, 0.864 P_2: 1.762, 3.619	
$T_{i,p}$(h)	P_1:19.271, 25.115, 24.712, 0, 24.800 P_2:118.229, 4.305, 16		P_1: 44.282, 37.5, 25.115, 24.712, 24.8 P_2: 16, 4.305, 100	

The results from Table 5 indicate as expected that the monolithic model for the iPSC has inferior performance when compared to the decomposed approach. As far as the comparison between TSP and the time slot formulation (T-S) is concerned, even though the integration through the TSP results in larger number of variables and constraints (because of the different linking constraints employed for the case of TSP), the TSP model needs less than half the number of binary variables to model the scheduling decisions. This advocates towards the better computational performance of the TSP over the T-S formulation for the iPSC. Moreover, despite the integration, suboptimal solutions may be computed because of the nonconvex nature of the problem. From a scheduling point of view the solution is suboptimal, since the monolithic iPSC chooses to perform a changeover between the adjacent planning periods even though product E is manufactured in both weeks and also the transition among products are not the optimal ones. In the solution computed by the monolithic approach we note that the transition times are not the minimum ones and this is because of the difficulty to identify the best possible transition due to the combinatorics involved. For example, in the first planning period the transition from A to D instead of 25.72h which is minimum transition time is computed as 57.88h and that results in not sufficient production time for A and backlog of the related demand.

One could argue that the solution of the decomposed iPSC is affected by the approximation involved in the metamodels. For that reason, the monolithic TSP model was solved again with all the binary decision fixed based on the solution of the decomposed iPSC and as expected the solutions computed among the two are identical as shown in Table 6.

Table 6: Results of the SISO CSTR case study with fixed sequencing decisions from the decomposed iPSC

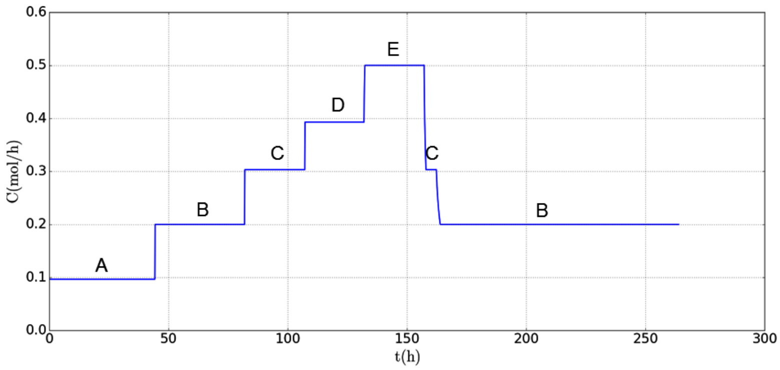
Model	Monolithic TSP	Decomposed iPSC
Type	MINLP	MILP (TSP)
Constraints	8,557	277
Cont. Var.	10,841	241
Binary Var.	105	105
Solver	SBB/CONOPT3	CPLEX 12.6.1
Profit ($)	9161172.25	9190688.58
CPU (s)	148.32	0.078
Optimal Schedule	P1: A→B→C→D→E P2: E→C→B	P1: A→B→C→D→E P2: E→C→B
$T^{trans}_{i,j,p}$(h)	P_1: 0.474, 0.575, 0.687, 1.944 P_2: 3.965, 8.142	P_1: 0.211, 0.256 , 0.305, 0.864 P_2: 1.762, 3.619
$T_{i,p}$(h)	P_1: 35.372, 37.5, 25.115,24.712, 24.8 P_2: 16, 4.305, 100	P_1: 44.282, 37.5, 25.115, 24.712, 24.8 P_2: 16, 4.305, 100

Table 6 shows that indeed the solution computed by the decomposed iPSC is correct and feasible for the original monolithic model. Notice, that even with all the binary variables fixed, it takes approximately 150s for SBB to compute the solution of the MINLP. It appears that the main bottleneck in the monolithic iPSC is the nonconvex DO part where the transition times are treated as decision variables. From a mathematical perspective this results in nonconvex bilinear terms which require a global optimisation scheme, e.g. the use of a spatial branch and bound. The comparative profit breakdown of the two solutions is given in Table 7.

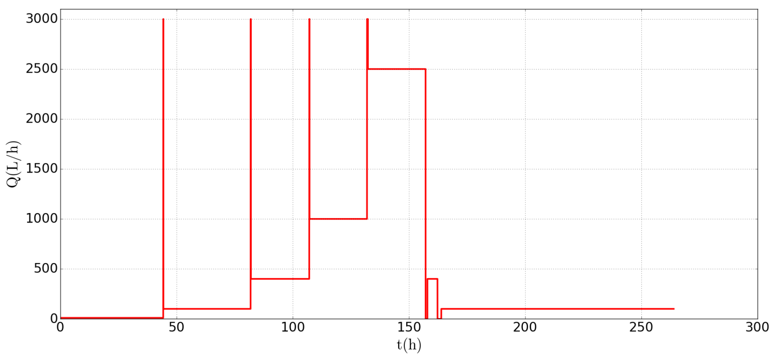
	Monolithic TSP	Decomposed iPSC
Sales ($)	10784287	10791000
Operational cost ($)	22437.6	22442
Inventory cost ($)	0	0
Transition cost ($)	67609.65	51143.4
Production cost ($)	1526354.4	1526726
Backlog cost ($)	6713.1	0

Table 7: Comparative cost breakdown of iPSC solution for the SISO case study

Figure 6, depicts the production plan computed in terms of the evolution of the state of the system and control input.



(a) Dynamic profile of the reactant's concentration over the planning horizon for the SISO CSTR case study



(b) Dynamic profile of the reactant's flowrate over the planning horizon for the SISO CSTR case study

Figure 6: Dynamic interpretation of the production plan for the SISO CSTR case study

Next, the same example is examined but this time, the discretisation of the time DO part is performed with 45 finite elements and 3 collocation point as design parameters for the OCFE. By doing so, the trade-off between the degree of the discretisation scheme and the optimal solution is under investigation. The minimum transition times and linear metamodels are computed again, using CONOPT3 and it takes 10.65s to converge. Table 8, provides the minimum transition times and as can be noticed the transition times are improved when compared to the ones computed with 20 finite elements.

Table 8: Minimum transition times for the SISO CSTR case study with OCFE of 45 finite elements and 3 collocation points

$\tau_{i,j}^{min}$ (h)	**A**	**B**	**C**	**D**	**E**
A	-	0.208	0.46	0.761	1.613
B	20.709	-	0.252	0.552	1.414
C	24.463	3.569	-	0.303	1.162
D	25.388	4.682	1.212	-	0.852
E	26.01	5.307	1.738	0.67	-

The monolithic and decomposed iPSC are solved again in GAMS and the results are provided in Table S2. Increasing the number of finite elements employed for the discretisation of the continuous dynamics on the one hand can potentially lead to more profitable operation but it also exacerbates the computational burden associated with the monolithic solution of the iPSC. Even in that case though, as observed in Table S2 the solution of the monolithic formulation does not guarantee that the benefits of the integration can be exploited. Similar to the previous results, where the OCFE was employed with 20 finite elements, because of the nonconvexity that characterises the problem again longer transition times and unnecessary changeovers between products occur that hindering the potential benefits of the integration. On the contrary, solving the corresponding DOs offline does not result to exhaustive computational times and the decomposed iPSC framework does not get affected performance-wise. Finally, we consider variable planning horizon and compare the performance between the TSP and

T-S formulation for the decomposed iPSC. As shown in Table S3, as the planning horizon increases the TSP model for the decomposed iPSC outperforms the T-S model. For the case of planning horizon of 12 weeks, for the same solution, TSP decomposed iPSC takes 4.4s while the T-S decomposed iPSC needs 3440.21s.

3.2 MIMO multi-product CSTR

The next case study examines the iPSC of a non-isothermal MIMO CSTR where the decomposition reaction of the form A→R takes place under the kinetic law: $-\mathscr{R}_b = \mathrm{k_r C_b}$. The reaction is exothermic and as such a cooling jacket is used; further details about the kinetics and design can be found in the book of Camacho and Alba[31]. The system is controlled through the flow rate of the liquid ($\mathrm{F_l}$) and the coolant ($\mathrm{F_c}$) while the corresponding states are the concentration of the decomposition product ($\mathrm{C_b}$) and the temperature of the liquid ($\mathrm{T_l}$). The calculation of the steady state conditions is carried out in an offline step and the related results are given in Table **??**. The utility price for the coolant $\mathrm{F_c}$ is \$10/m^3 while cost of product liquid $\mathrm{F_l}$ is \$10/m^3. The dynamic model of the system is derived based on the mass and energy balances as shown in eq. (54)-(55), respectively where the concentration of reactant A is assumed to be constant. Further details about the system can be found in the book of Camacho and Alba[31] and in Zhuge and Ierapetritou[14]. The rest of the data about the case study are given in Tables S4-S5; the cost of backlog is calculated as half of the selling price of the related product.

$$\frac{\mathrm{d(V_l C_b)}}{\mathrm{dt}} = \mathrm{V_l k_r (C_{a0} - C_b) - F_l C_b} \tag{54}$$

$$\frac{\mathrm{d(V_l \rho_l C_{pl} T_l)}}{\mathrm{dt}} = \mathrm{F_l \rho_l C_{pl} T_{l0} - F_l \rho_l C_{pl} T_l + F_c \rho_c C_{pc} (T_{c0} - T_c) + V_l k_r (C_{a0} - C_b) H} \tag{55}$$

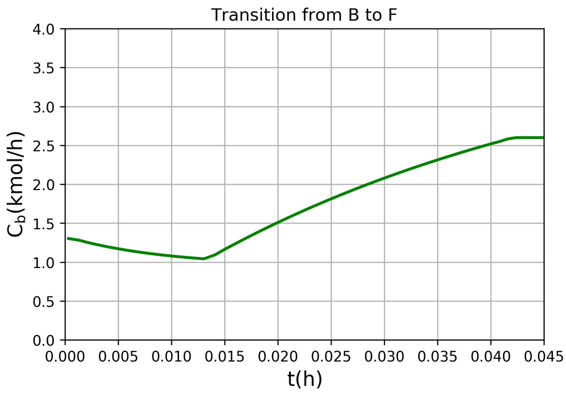
Table 9: Design parameters of the MIMO multi-product CSTR case study

k_r reaction constant	26 $\frac{1}{h}$
V_l volume of the tank	24L^3
ρ_l liquid density	800 $\frac{kg}{m^3}$
ρ_c coolant density	1000 $\frac{kg}{m^3}$
C_{pl} specific heat of liquid	3 $\frac{kJ}{kg \cdot K}$
C_{pc} specific heat of coolant	4.19 $\frac{kJ}{kg \cdot K}$
T_{l0} entering liquid temperature	283K
T_{c0} inlet coolant temperature	273K
T_c outlet coolant temperature	303K
C_{a0} initial concentration of the reactant	4 $\frac{mol}{L}$

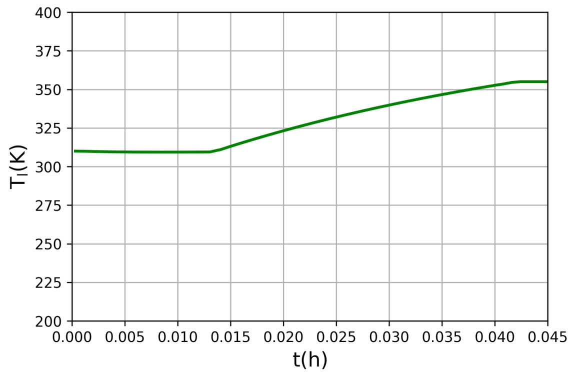
The minimum transition times as calculated by the offline DO, for discretisation with OCFE with 20 finite elements and 3 collocation points, are shown in Table 10. The coefficients for the linear metamodels that correlate transition time and cost are also given in Table S6. The transition times computed indicate system's fast dynamics where rapid changeovers between manufacturing conditions are achieved. This particular instance is very insightful as ideally, one would like to be in a position to have the solution of the integrated problem at hand in times faster than the transition times. This is because, assuming that the system is subject to disturbances at the level of process dynamics, then deviation from the precomputed transition time/profile may lead to economic loss of the process. The dynamic response of the system as shown in Figure 7, for the case of transition from product B to product F, the fast transitions are achieved with rapid rate of change of the manipulated variables while the profiles of the state variables remain rather smooth.

Table 10: Minimum transition times between products for the MIMO case study

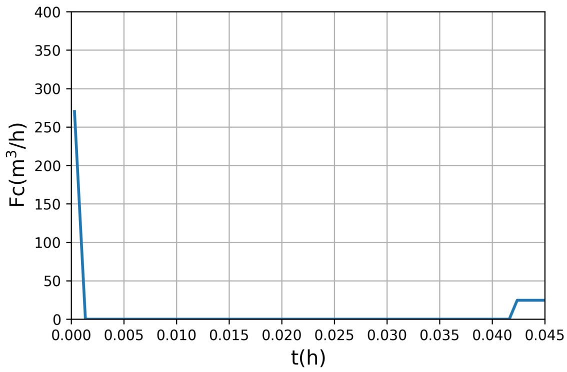
$\tau_{\mathrm{i,j}}^{\mathrm{min}}$ (h)	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**H**
A	-	0.013278	0.028574	0.051289	0.044191	0.052304	0.036262	0.067748
B	0.018478	-	0.01841	0.042275	0.033493	0.042478	0.032414	0.055689
C	0.024308	0.005830	-	0.030435	0.018565	0.026075	0.027433	0.048667
D	0.028820	0.010342	0.004997	-	0.011364	0.014089	0.025556	0.041064
E	0.032483	0.014105	0.008174	0.032077	-	0.022706	0.024201	0.029812
F	0.033071	0.014592	0.008761	0.023927	0.001137	-	0.025253	0.02738
G	0.034146	0.021649	0.038830	0.062261	0.054110	0.062779	-	0.076709
H	0.035896	0.017670	0.011920	0.037532	0.011257	0.030208	0.024550	-



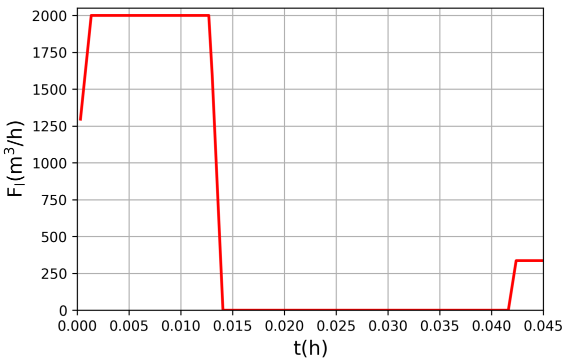
(a) Dynamic profile of the concentration of the decomposition product



(b) Dynamic profile of the temperature of the liquid



(c) Dynamic profile of the flow rate of the coolant



(d) Dynamic profile of the flow rate of the liquid

Figure 7: Dynamic response of the system for the transition from B to F

Formulating and solving the monolithic and decomposed iPSC the results shown in Table 11, are computed.

Table 11: Results for the MIMO CSTR case study for planning horizon of 2 weeks. OCFE with 20 finite elements and 20 collocation points was employed for the discretisation of the DO part.

Model	Monolithic TSP	Monolithic T-S	Decomposed iPSC	
Type	MINLP		MILP (TSP)	MILP (T-S)
Constraints	45,703	8,965	647	4,157
Cont. Var.	60,465	10,865	601	3,361
Binary Var.	240	1,152	240	1,152
Solver	SBB/CONOPT3		CPLEX 12.6.1	
Profit ($)	3075778.96		7710974.76	
CPU (s)	660.15	832.25	0.765	50.857
Optimal Schedule	P_1 : B → H → A → G P_2 : B → C → G → A → F		P1: D→F→E→C→B→A P2: A→B→C→D→F→E→H→G	
$T^{trans}_{i,j,p}$(h)	P_1: 0.057, 0.212, 0.037 P_2: 0.586, 0.019, 0.028, 0.796, 0.053		P_1: 0.014, 0.001, 0.008, 0.018 P_2: 0.013, 0.018, 0.030, 0.014, 0.001, 0.030, 0.025	
$T_{i,p}$(h)	P_1: 22.862, 6.476, 28.490, 57.648 P_2: 1.429, 2.849, 12.464, 1.959, 95.663		P_1: 24.038, 85.034, 4.856, 24.712, 2.671, 22.862, 28.490 P_2: 1.959, 1.429, 0.178, 4.006, 10.629, 66.369, 6.476, 70.112	

The multi-product MIMO CSTR case study, differs from the SISO CSTR case study that was previously studied in the following two: (1) it has increased dimensionality in terms of control and state variables and (2) the number of products is also increased from 5 to 8. The first difference, affects mostly the DO part of the iPSC while the second affects the combinatorial nature on the level of planning-scheduling of the iPSC. This effect, becomes apparent after the observation of the results in Table 11. The solution computed through the monolithic approach, is clearly suboptimal because not only the transition times computed are not the minimum possible ones but also because there is a number of inconsistencies at a planning and scheduling level. More specifically, again a changeover occurs across the adjacent planning weeks which should not have occurred since product B is produced in both weeks; next, the entire available time is not consumed especially in week 1 where a great amount of demand, e.g. for product E, is backlogged despite the availability of processing time.

Because of the great difference computed between the two solution approaches as shown in Table 11, again the integer decisions as computed by the decomposed approach are fixed in the monolithic model and it is solved again in “reduced space”. Not surprisingly, with exception some of transition times which were computed with larger values by the monolithic model, the solutions are identical in terms of planning and scheduling decision while the dynamic profiles are the same as well. In Figure 8, a comparative graph with the flowrate of the coolant as computed by the monolithic and the decomposed model can be envisaged.

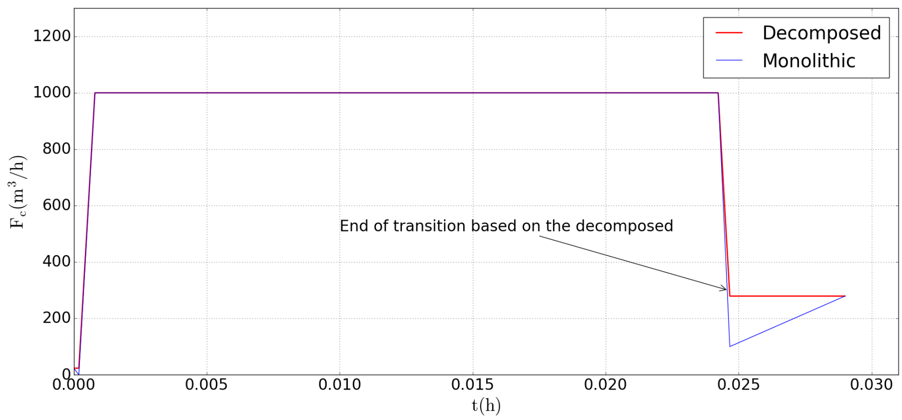


Figure 8: Comparative graph of the coolant flowrate ($F_c = f(t)$) as computed by the decomposed and the monolithic solution approach

Figure 8, shows that the monolithic approach computes a less optimal solution for the transition from product H to product G as in the beginning the first control move is 0 and then reaches the value of 1000 m^3/h.

Next, the computational performance of the T-S and TSP models for the decomposed iPSC is compared based on three different planning periods, i.e. 4 weeks, 6 weeks and 12 weeks. The related demand over the planning period for each product is given in Table S7.

As shown in Table S8, increasing the number of products has a significant impact on the computational performance of both models since the number of binary variables is increased. However, even in that case the computational performance of the TSP formulation is better than the one achieved by the T-S formulation.

3.3 MMA polymerisation process

Next, the iPSC of the isothermal methyl-methacrylate polymerisation process[32] is considered, where different polymer grades are produced. The free radical polymerisation reaction takes place in a CSTR isothermally, with azobisisobutyronitrile as initiator and toluene as the solvent. Graphically the system under consideration is shown is Figure 9.

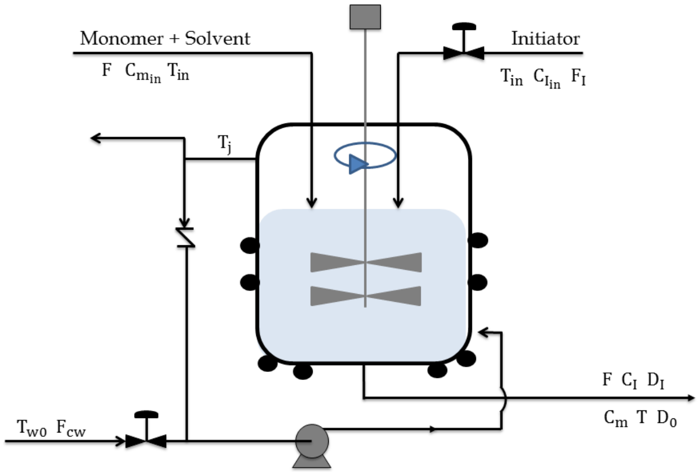


Figure 9: MMA polymerisation reactor

$$\frac{dC_m}{dt} = -(k_p + k_{fm})\sqrt{\frac{2f^* k_I}{k_{T_d} + k_{T_c}}} C_m \sqrt{C_I} + \frac{F(C_m^{in} + C_m)}{V} \tag{56}$$

$$\frac{dC_I}{dt} = -k_I C_I + \frac{F_I C_I^{in} - F C_I}{V} \tag{57}$$

$$\frac{dD_0}{dt} = (0.5 k_{T_c} + k_{T_d}) \frac{2f^* k_I}{k_{T_d} + k_{T_c}} C_I + k_{fm} \sqrt{\frac{2f^* k_I}{k_{T_d} + k_{T_c}}} C_m \sqrt{C_I} - \frac{F D_0}{V} \tag{58}$$

$$\frac{dD_I}{dt} = M_m (k_p + k_{fm}) \sqrt{\frac{2f^* k_I}{k_{T_d} + k_{T_c}}} C_m \sqrt{C_I} - \frac{F D_I}{V} k_p \tag{59}$$

$$y = \frac{D_I}{D_0} \tag{60}$$

$$u = F_I \tag{61}$$

The dynamic model of the system is derived based on the following assumptions[32]: (i) constant density and heat capacity of the reacting mixture and the coolant, (ii) insulated reactor and cooling system, (iii) no polymer in the inlet streams, (iv) no gel effect caused by the low polymer conversion, (v) constant reactor volume, (vi) negligible flow rate of the initiator solution compared to the flow rate of the monomer stream, (vii) negligible inhibition and chain transfer to solvent reactions, (viii) quasi-steady state and long chain hypothesis. Data about the kinetic and design information of the MMA case study are given in Table 12. The system consists of four different states, namely: $\mathrm{C_m}$ is the monomer concentration, $\mathrm{C_I}$ represents the concentration of the initiator, $\mathrm{D_0}$ denotes the molar concentration of dead polymer chain while $\mathrm{D_I}$ the corresponding mass concentration.

Table 12: Data for MMA case study

$\mathrm{Q_m}$	1	Monomer feed stream [$\mathrm{m^3/h}$]
V	0.1	Reactor volume [$\mathrm{m^3}$]
$\mathrm{C_{i_{in}}}$	8	Feed stream initiator concentration [$\mathrm{kmol/m^3}$]
$\mathrm{M_m}$	100.12	Monomer molecular weight [kg/kmol]
$\mathrm{C_{m_{in}}}$	6	Feed stream monomer concentration [$\mathrm{kmol/m^3}$]
f^*	0.58	Initiator efficiency
$\mathrm{k_{tc}}$	1.3281×10^{10}	Termination by coupling rate constant [$\mathrm{m^3/(kmol\cdot h)}$]
$\mathrm{k_{td}}$	1.093×10^{11}	Termination by disproportion rate constant [$\mathrm{m^3/(kmol\cdot h)}$]
$\mathrm{k_i}$	1.0255×10^{-1}	Initiation rate constant [1/h]
$\mathrm{k_p}$	2.4952×10^{6}	Propagation rate constant [[$\mathrm{m^3/(kmol\cdot h)}$]
$\mathrm{k_{fm}}$	2.4522×10^{3}	Chain transfer to monomer rate constant [$\mathrm{m^3/(kmol\cdot h)}$]

The system is controlled through the manipulation of the initiator flow rate ($\mathrm{F_I}$) while the measurable output (y) is the average molecular weight of each polymer grade. Based on the multiple steady states that the system exhibits[33], products of different quality can be produced. In the present work 5 different polymer grades are produced and the corresponding information about the steady state operating conditions are given in Table 13 while the related demand and cost data are given in Table S9. Note that the backlog cost is calculated as $\mathrm{CB_{i,c}} = 0.5\cdot\mathrm{P_i}$ and the inventory cost is $\mathrm{C_i^{inv}} = 0.1(\$/\mathrm{m^3}\cdot\mathrm{h})$.

Table 13: Steady state operating conditions for the MMA products

Products	C_m^{ss}(kmol/m^3)	C_I^{ss}(kmol/m^3)	D_0^{ss}(kmol/m^3)	D_I^{ss}(kg/m^3)	y(kg/kmol)	F_I(m^3/h)
A	3.078	0.148	0.0195	292.546	15000	0.2048
B	3.725	0.0615	0.0091	227.699	25000	0.0847
C	3.978	0.0426	0.0067	202.380	30000	0.0586
D	4.201	0.0302	0.0051	180.064	35000	0.0416
E	4.583	0.0157	0.00315	141.866	45000	0.0217

The dynamic optimisation of the corresponding system is rather demanding as it results in numerical issues, which stem from the different numerical scales associated with the state and control variables. Following the proposed framework, first the pairwise minimum transition times are computed offline resulting in 20 DO problems. The DO problems are further discretised using OCFE with 3 collocation points and 20 finite elements and the corresponding NLP problem are formulated and solved in GAMS using BARON 14.4 and CONOPT3 as solvers. The results of the minimum transition times are given in Table 14 while an example of the profiles of the control input and system output during the transition from product E to D is shown in Figure S2. The coefficients for the linear metamodels for the MMA case study can be found in Table S10.

Table 14: Minimum transition times for the MMA case study

$\tau_{i,j}^{min}$ (h)	**A**	**B**	**C**	**D**	**E**
A	-	3.64	4.45	5.18	6.51
B	2.65	-	2.61	3.58	5.13
C	2.84	1.28	-	2.65	4.45
D	2.93	1.48	1.17	-	3.72
E	3.00	1.61	1.40	1.24	-

It is should be mentioned that both BARON and CONOPT3 converge to the same solution but despite the fact that CONOPT3 is much faster it requires the provision of a good initialisation point as noted while performing the numerical experiments. The computational statistics are given in Table

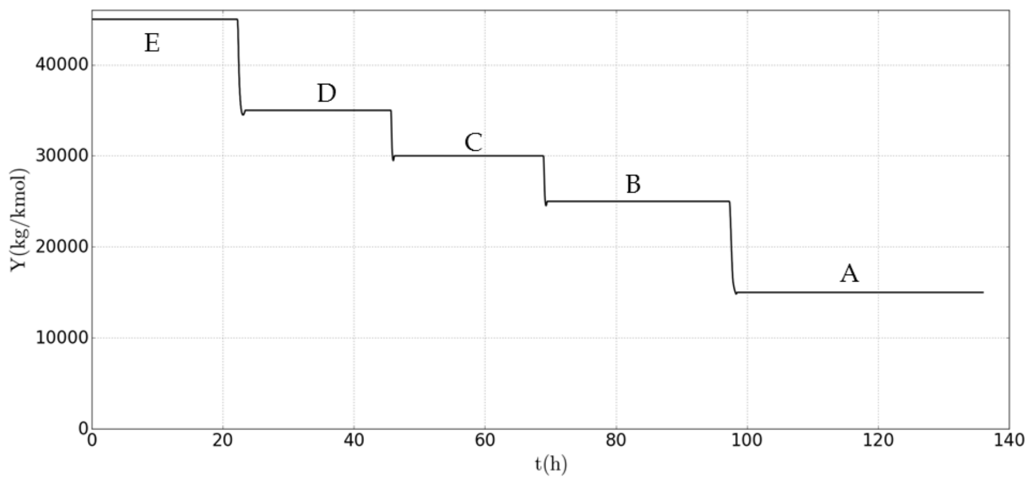
S11. The same problems were solved employing OCFE with 45 finite elements with slightly improved results computed which for the sake of space are not reported herein.

After the minimum transition times have been computed, with transition time up to three times the minimum one, i.e. $\mathrm{T}^{\mathrm{trans}}_{\mathrm{i,p}} \in [\tau^{\mathrm{min}}_{\mathrm{i,j}}, 3\tau^{\mathrm{min}}_{\mathrm{i,j}}]$ a series of optimisation problems are solved with the objective to minimise the corresponding transition cost, i.e. the utilisation of control input. Once the linear meta-models have been computed offline, both the monolithic and the decomposed one are formulated and solved in GAMS and the corresponding statistics are given in Table 15.

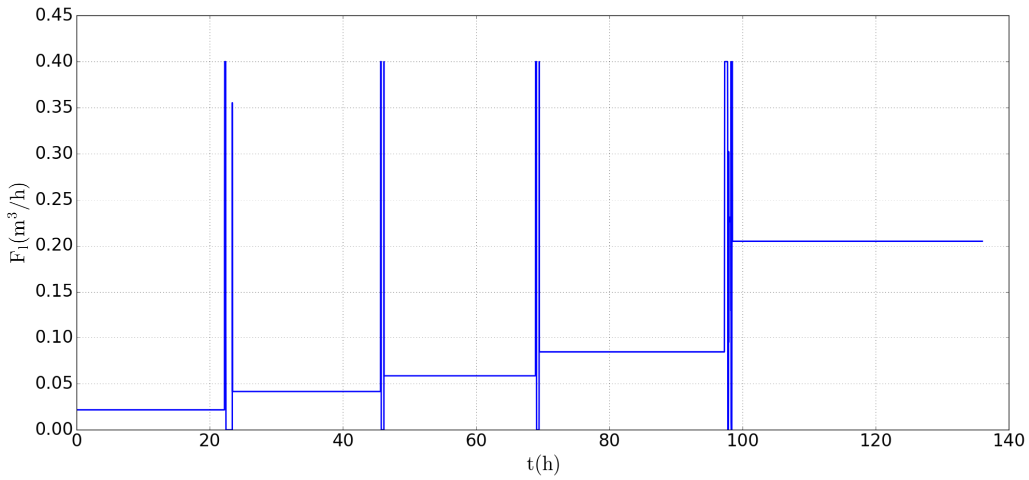
Table 15: Results of the computational performance between the monolithic and the decomposed integrated model using the proposed TSP and the time-slot (T-S) based formulation for the MMA case study

Model	**Monolithic TSP**	**Monolithic T-S**	**Decomposed TSP**	**Decomposed T-S**
Planning Horizon	2 weeks			
Type	MINLP	MINLP	MILP	MILP
Constraints	35,067	7,890	287	1,083
Cont. Var.	37,767	10,811	236	951
Binary Var.	105	300	105	300
Solver	SBB/CONOPT3		CPLEX 12.6.1	
Profit ($)	11423.98	11423.98	15439.57	15439.57
CPU (s)	8253.64	10,323.3	0.39	1.5
Gap (%)	0.26295	0.26295	0	0

In Table S12, the decision made by the decomposed iPSC are shown while in Figure 10 the systems-dynamic interpretation of the corresponding schedule for the first planning period can be envisaged.



(a) Dynamic profile of the output (y) for the first planning period of the MMA case study



(b) Dynamic profile of the initiator flowrate (F_I) for the first planning period of the MMA case study

Figure 10: Dynamics interpretation of the optimal production schedule for the first planning period of the MMA case study

In Table S13, the decision computed by the monolithic approach are given in more details. Studying Table S13, justifies why the solution computed by the monolithic models (both the TSP and the T-S) is clearly suboptimal when compared to the decomposed one. First similarly to the previous case studies, from a scheduling perspective unnecessary change-over occurs between planning period 1 and 2, as A is produced in both periods and the change-over sequence within each planning period differs from the one computed by the decomposed one. The latter, results in less available production time and an amount of demand to be backlogged, thus incurring additional costs.

Another interesting observation is the change-over performed at the second planning period from A to E, from the decomposed iPSC. One by reading Table 14, would probably expect to have a changeover between A and B as the transition time is less; however, the optimiser chooses the transition between A and E and this is due to the less transition cost involved. This particular instance, stands for a very clear example of where optimal control, planning and scheduling interconnect and how the proposed decomposition captures these interdependences without strenuous computational times.

In order to demonstrate the computational potential of the proposed decomposition the same case study was examined with planning horizons of 4, 6 and 12 weeks and a comparison between the TSP and T-S formulation was conducted. As shown in Table 16, for short planning horizons the TSP and T-S perform similarly but as larger planning horizons are considered the TSP outperforms the T-S formulation. This can be justified by both the less number of equations and variables generated and the symmetry breaking constraints used.

Table 16: Comparison between the decomposed TSP and T-S formulation for varying planning horizons

Planning horizon	4 weeks		6 weeks		12 weeks	
Decomposed Model	**TSP**	**T-S**	**TSP**	**T-S**	**TSP**	**T-S**
Type	MILP	MILP	MILP	MILP	MILP	MILP
Constraints	583	2,185	879	3,287	1,767	6,593
Cont. Var.	516	1,901	776	2,851	1,556	5,701
Binary Var.	235	600	365	900	755	1,800
Solver	CPLEX 12.6.1					
Profit ($)	29563.4	29563.4	45831.07	45831.07	71570.46	71570.46
CPU (s)	0.328	235.031	1.654	1700	9.251	3600
Gap (%)	0	0	0	0	0	0.03

Finally, the case of multiple customers for planning horizon of 8 weeks is examined with a total of 10 customers. The related computational results are given in Table S14.

4 Concluding remarks

In the present work we dealt with the integrated Planning, Scheduling and optimal Control (iPSC) of continuous manufacturing processes. A TSP based model is employed for the decision on the levels of planning and scheduling and was compared to the time-slot based models adapted by the majority of the research works for the integrated problem. As shown from the three different case studies, the TSP and T-S based integration perform similarly for small planning horizons while for larger planning horizons the TSP based model outperforms the T-S considerably. New features for the integrated problem are studied such as multiple customers, inventory capacity as well as backlog and idle production time within the planning period are allowed. Aiming to reduce the computational complexity of the iPSC, a decomposition based on linear metamodels was proposed and tested under the assumption that we account for the open loop performance of the underlying dynamic system. The linear metamodels, associate the transition cost with the transition time between the different products manufactured. Computational studies indicate that when disturbances are not considered at the level of control then the solutions computed from the decomposed iPSC and the monolithic when solved to global optimality are equivalent. Future work in our group is directed towards the extension of the proposed framework for the closed loop implementation of the solution computed by the iPSC so as to account for systematic disturbances.

Acknowledgments

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Supporting Information

The Supporting Information is available free of charge via the Internet at http://pubs.acs.org/.

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Appendix A

The model proposed by Erdirik-Dogan and Grossmann [20], for the integration of planning and scheduling of single stage multi-product continuous processes serves as a basis for the slot based iPSC formulations that have been proposed in the literature. The model is a multi-period MILP in continuous time representation where the number of slots available within a planning period is equal to the number of products produced by the process.

Nomenclature for E-D&G model

Indices	
i, j	products : $\mathrm{i, j = 1, \ldots, N}$
p	planning periods : $\mathrm{p = 1, \ldots, N_p}$
s	time slots : $\mathrm{s = 1, \ldots, N_s}$
Parameters	
$\mathrm{D_{i,p}}$	Demand of product i in period p
$\mathrm{H_t}$	Duration of the $\mathrm{p^{th}}$ planning period
$\mathrm{HT_p}$	Time at the end of the planning horizon p
$\mathrm{INV0_{i1}}$	Initial inventory of product i
M	Big − M constraint parameter
$\mathrm{N_{i,p}}$	Maximum number of products per planning period
$\mathrm{r_i}$	production rate of product i
τ_{ij}	Transition time from product i to j
Continuous Variables	
$\mathrm{Area_{ip}}$	Overestimating area below the graph relating inventory during period p
$\mathrm{INV_{ip}}$	Inventory level of product i at the end period p
$\mathrm{INVO_{ip}}$	Inventory level of product i after the demand of period p is met
$\mathrm{NY_{ip}}$	Number of slots in planning period p that product i occupies
$\mathrm{\tilde{q}_{isp}}$	Production amount of product i in slot s of period p
$\mathrm{q_{ip}}$	Total production amount of product i in period p
$\mathrm{S_{ip}}$	Sales level of product i in period p
$\mathrm{T^s_{sp}}$	Starting time of slot s in planning period p
$\mathrm{T^e_{sp}}$	Ending time of slot s in planning period p
$\tilde{\theta}_{\mathrm{isp}}$	Production time of product i in slot s of period p
θ_{ip}	Total production time of product i in period p
Binary Variables	
$\mathrm{W_{isp}}$	1, if product i is assigned to slot s of period p; 0, otherwise
$\mathrm{Y_{ip}}$	1, if product i is assigned to period p; 0, otherwise
$\mathrm{Z_{ijsp}}$	1, if product i precedes j, produced in timeslot s, in period p; 0, otherwise
$\mathrm{Z'_{ijp}}$	1, if product i precedes j, produced at the end of period p; 0, otherwise

Mathematical formulation

1. Assignment and Processing time:

$$\sum_{i} \mathrm{W_{isp}} = 1 \qquad \forall \mathrm{s} \in \mathrm{N_s};\ \mathrm{p} \in \mathrm{N_p} \tag{A.1}$$

$$0 \leq \tilde{\theta}_{\mathrm{isp}} \leq \mathrm{W_{isp}} \cdot \mathrm{H_p} \qquad \forall \mathrm{i} \in \mathrm{I};\ \forall \mathrm{s} \in \mathrm{N_s};\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.2}$$

$$\theta_{\mathrm{ip}} = \sum_{s} \tilde{\theta}_{\mathrm{isp}} \qquad \forall \mathrm{i} \in \mathrm{I};\ \mathrm{p} \in \mathrm{N_p} \tag{A.3}$$

$$\theta_{\mathrm{ip}} \leq \mathrm{Y_{ip}} \cdot \mathrm{H_p} \qquad \forall \mathrm{i} \in \mathrm{I};\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.4}$$

2. Production rates:

$$\tilde{\mathrm{q}}_{\mathrm{isp}} = \mathrm{r_i} \tilde{\theta}_{\mathrm{isp}} \qquad \forall \mathrm{i} \in \mathrm{I};\ \forall \mathrm{s} \in \mathrm{N_s};\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.5}$$

$$\mathrm{q_{ip}} = \sum_{s} \tilde{\mathrm{q}}_{\mathrm{isp}} \qquad \forall \mathrm{i} \in \mathrm{I};\ \mathrm{p} \in \mathrm{N_p} \tag{A.6}$$

3. Transition within production periods:

$$\mathrm{Z_{ijsp}} \geq \mathrm{W_{isp}} + \mathrm{W_{j,s+1,p}} - 1 \qquad \forall \mathrm{i,j} \in \mathrm{I};\ \forall \mathrm{s} = 1, \ldots, \mathrm{Ns} - 1;\ \forall \mathrm{p} \in \mathrm{N_p},\ \mathrm{i} \neq \mathrm{j} \tag{A.7}$$

4. Transition across production periods:

$$\mathrm{Z'_{ijp}} \geq \mathrm{W_{iN_sp}} + \mathrm{W_{j1,p+1}} - 1 \qquad \forall \mathrm{i,j} \in \mathrm{I};\ \forall \mathrm{p} = 1, \ldots, \mathrm{N_p} - 1,\ \mathrm{i} \neq \mathrm{j} \tag{A.8}$$

5. Timing relations:

$$\mathrm{T^s_{11}} = 0 \tag{A.9}$$

$$\mathrm{T^e_{sp}} = \mathrm{T^s_{sp}} + \sum_{i} \tilde{\theta}_{\mathrm{isp}} + \sum_{i}\sum_{j} \tau_{\mathrm{ij}} \mathrm{Z_{ijsp}} \qquad \forall \mathrm{s} \in \mathrm{N_s};\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.10}$$

$$\mathrm{T^e_{N_sp}} + \sum_{i}\sum_{j} \tau_{\mathrm{ij}} \mathrm{Z'_{ijp}} = \mathrm{T^s_{1,p+1}} \qquad \forall \mathrm{p} = 1, \ldots, \mathrm{N_p} - 1 \tag{A.11}$$

$$\mathrm{T^e_{sp}} = \mathrm{T^e_{s+1,p}} \qquad \forall \mathrm{s} = 1, \ldots, \mathrm{N_s} - 1;\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.12}$$

$$\mathrm{T^e_{N_sp}} \leq \mathrm{HT_p} \qquad \forall \mathrm{p} \in \mathrm{N_p} \tag{A.13}$$

6. Inventory calculation:

$$\mathrm{INV_{ip}} = \mathrm{INV0_{i1}} + \sum_{s} \mathrm{r_i} \tilde{\mathrm{q}}_{\mathrm{isp}} \qquad \forall \mathrm{i} \in \mathrm{I};\ \mathrm{p} = 1 \tag{A.14}$$

$$\mathrm{INV_{ip}} = \sum_{s} \mathrm{r_i} \tilde{\mathrm{q}}_{\mathrm{isp}} \qquad \forall \mathrm{i} \in \mathrm{I};\ \forall \mathrm{p} \in \mathrm{N_p} - \{1\} \tag{A.15}$$

$$\mathrm{INVO_{ip}} = \mathrm{INV_{ip}} - \mathrm{S_{ip}} \qquad \forall \mathrm{i} \in \mathrm{I};\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.16}$$

$$\mathrm{Area_{ip}} \geq \mathrm{INVO_{i,p-1}} \mathrm{H_p} + \mathrm{r_i} \theta_{\mathrm{ip}} \mathrm{H_p} \qquad \forall \mathrm{i} \in \mathrm{I},\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.17}$$

7. Sales satisfaction:

$$\mathrm{S_{ip}} \geq \mathrm{D_{ip}} \qquad \forall \mathrm{i} \in \mathrm{I},\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.18}$$

8. Symmetry breaking constraints:

$$\mathrm{NY_{ip}} = \sum_{\mathrm{s}} \mathrm{W_{isp}} \qquad \forall \mathrm{i} \in \mathrm{I},\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.19}$$

$$\mathrm{Y_{ip}} \geq \mathrm{W_{isp}} \qquad \forall \mathrm{i} \in \mathrm{I},\ \forall \mathrm{s} \in \mathrm{N_s},\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.20}$$

$$\mathrm{Y_{ip}} \leq \mathrm{NY_{ip}} \leq \mathrm{N_{ip}Y_{ip}} \qquad \forall \mathrm{i} \in \mathrm{I},\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.21}$$

$$\mathrm{NY_{ip}} \geq \mathrm{N_{ip}} - [(\sum_{\mathrm{i}} \mathrm{Y_{ip}}) - 1] - \mathrm{M}(1 - \mathrm{W_{isp}}) \qquad \forall \mathrm{i} \in \mathrm{I},\ \forall \mathrm{s} \in \mathrm{N_s},\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.22}$$

$$\mathrm{NY_{ip}} \leq \mathrm{N_{ip}} - [(\sum_{\mathrm{i}} \mathrm{Y_{ip}}) - 1] + \mathrm{M}(1 - \mathrm{W_{isp}}) \qquad \forall \mathrm{i} \in \mathrm{I},\ \forall \mathrm{s} \in \mathrm{N_s},\ \forall \mathrm{p} \in \mathrm{N_p} \tag{A.23}$$

Abbreviations	**Meaning**
APC	Advanced Process Control
BVP	Boundary Value Problem
DO	Dynamic Optimisation
EWO	Enterprise Wide Optimisation
ISA	International Society of Automation
iPSC	integrated Planning Scheduling and Control
iSC	integrated Scheduling and Control
MIDO	Mixed Integer Dynamic Optimisation
MILP	Mixed Integer Linear Programming
MIMO	Multiple Input Multiple Output
MINLP	Mixed Integer Nonlinear Programming
MMA	methyl-methacrylate
MPC	Model Predictive Control
NLP	Nonlinear Programming
NMPC	Nonlinear Model Predictive Control
OCFE	Orthogonal Collocation on Finite Elements
RHS	right-hand side
SBM	time Scale Bridging Model
SISO	Single Input Single Output
T-S	Time-Slot
TSP	Travelling Salesman Problem

Table 17: Index of abbreviations

Indices/Sets	
c =	costumers
cp/cpp =	collocation points
fe =	finite elements
i,j =	products
m =	control inputs
n =	state variables
p =	planning periods
Parameters	
A1=	transition cost of raw materials
A2=	production cost of raw materials
B1=	linear estimation transition cost of raw materials
$\mathrm{C_m^{raw}}$=	raw material cost of the m-th control input
$\mathrm{CB_{ic}}$=	backlog cost of product i for costumer c
$\mathrm{C_i^{inv}}$=	inventory cost of product i
$\mathrm{C_i^{oper}}$=	operational cost of product i
$\mathrm{D_{cip}}$=	demand of product i from costumer c at the end of planning period p
$\mathrm{h^{ocfe}}$=	step size of the OCFE
iter =	iteration counter for the development of the linear metamodels
M =	big-M parameter
$\mathrm{N_{fe}}$=	cardinality of the set of finite elements
$\mathrm{n_{sample}}$=	total number of sampling points for the development of the linear metamodels
PROF =	profit
$\mathrm{P_i}$=	selling price of product i
$\mathrm{r_i}$	production rate
$\mathrm{roots_{cp}}$=	roots of the Lagrange orthogonal polynomial
$\mathrm{t^{max}}$=	maximum variance of the transition time for the development of the metamodels
$\mathrm{u_{mi}^{ss}}$=	m-th steady state value of the control variable for product i
$\mathrm{x_{ni}^{ss}}$=	n-th steady state value of the state variable for product i
$\mathrm{V_i^{min}/V_i^{max}}$=	lower and upper level of inventory for product i
α_{ij}=	slope coefficient for the linear metamodel for the transition form product i to j
β_{ij}=	intercept coefficient for the linear metamodel for the transition form product i to j
$\theta^{\mathrm{lo}}, \theta^{\mathrm{up}}$=	lower and upper bounds on production time
σ=	dynamic model parameters
$\tau_{\mathrm{ij}}^{\mathrm{min}}$=	minimum transition time from product i to product j
τ_{max}=	big value parameter used for exact linearisation
Φ_1=	revenue
Φ_2=	total operational cost
Φ_3=	total inventory cost
Φ_4=	total backlog cost
$\Omega_{\mathrm{cp,cp}}$	collocation matrix

Decision Variables

B_{cip}= backlog level of product i for costumer c at the end of planning period p

CT^{tran}_{ij}= transition cost from product i to j

$CT1_p$ = changeover crossover variable indicating the time elapsed in period p for a changeover that started in period p-1

$CT2_p$ = changeover crossover variable indicating the time elapsed in period p for a changeover that finishes in the next time period

E_{ip}= binary variable indicating assignment of product i to planning period p

F_{ip}= binary variable indicating the first product in planning period p

L_{ip}= binary variable indicating the last product in planning period p

O_{ip}= integer variable used as order index

Pr_{ip}= production level of product i at the end of planning period p

S_{cip}= sales level of product i to costumer c at the end of planning period p

T_{ip}= production time

$\tilde{t}_{ijpfecp}$= discretised time variable

T^{trans}_{ijp}= transition time from product i to j during planning period p

$T^{trans_{lin_1}}_{ijp}$= linearised transition time variable from product i to j during planning period p

$T^{trans_{lin_2}}_{ijp}$= linearised transition time variable from product i to j across planning period p

u^{in}_{mijp} initial value of the m-th control input for transition $i \rightarrow j$ during planning period p

$u^{ocfe}_{mijpfecp}$ discretised m-th control input for transition $i \rightarrow j$ during planning period p

u^{fin}_{mijp} final value of the m-th control input for transition $i \rightarrow j$ during planning period p

V_{ip} inventory level of product i at the end of planning period p

$\dot{x}_{nijpfecp}$ numerical value of the derivative for the n-th state for transition $i \rightarrow j$ during planning period p

x^{in}_{nijp} initial value of the n-th state variable for transition $i \rightarrow j$ during planning period p

$x^{ocfe}_{nijpfecp}$ discretised n-th state variable for transition $i \rightarrow j$ during planning period p

$x^{ocfe_{init}}_{nijpfe}$ discretised n-th state variable for transition $i \rightarrow j$ during planning period p at the beginning of finite element fe

x^{fin}_{nijp} final value of the n-th state variable for transition $i \rightarrow j$ during planning period p

Z_{ijp}=	binary variable indicating transition $i \rightarrow j$ during planning period p
Zf_{ijp}=	binary variable indicating transition between periods p - 1 and p from product i to j

Nomenclature

Contents