Dynamic Real-Time Optimization of Transitions in Industrial Polymerization Processes using Solution Models

J.V. Kadam[a], B. Srinivasan[b], W. Marquardt[1,a], D. Bonvin[b]

[a]Lehrstuhl für Prozesstechnik
RWTH Aachen University, Turmstr. 46
D-52064 Aachen, Germany
[b]Laboratoire d'Automatique
École Polytechnique Fédérale de Lausanne
CH-1015 Lausanne, Switzerland

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1 Introduction

The production of synthetic polymers exceeds 100 million tons per year worldwide with their many different grades and prices. While on the one hand the product specifications for high value products become tighter and tighter, on the other hand many of the specialty polymers are becoming commodities resulting lower profit margins, thus requiring an efficient and cost-effective production. Furthermore, the highly fluctuating demands of the global market call for a very flexible process operation with frequent changes in polymer grade, production load and product quality. Thus, for the polymer industries, the competitive edge will essentially come from the technologies that excel in controlling the polymer properties in a consistent way while concurrently and flexibly satisfying the market demand and improving the economical performance. Besides the economical aspects, the intrinsic characteristics of polymerization processes pose challenging problems of operation, control and optimization.

Three distinct types of operational problems in the polymer industry are usually encountered. The most common problem is the *quality control problem*. The task to be solved is to keep the quality relevant parameters at their desired setpoints despite disturbances, in order to stay within the bounds given for the desired end user properties. Disturbances here can either be general stochastic process disturbances, e.g. changing feed properties, but also disturbances forced on the process by the operational policy, e.g. changes of production load or product grades. The second problem, referred to as the *grade change problem*, actually corresponds to one of these disturbance scenarios. Most polymerization plants, even though being continuous plants, produce more than one distinct grade of polymer on one production line. These

[1]Corresponding author: Marquardt@LPT.RWTH-Aachen.de, +49/241/80 97002

grade changes tend to become more and more frequent due to tighter requirements given by market demands and supply chain optimization. During the transition from one grade to another the unit in most cases produces a certain amount of polymer not satisfying the quality requirements of either two grades which can then only be sold as low-value off-spec product. One major task for improving the economics of operation is to determine optimized operational trajectories which minimize the amount of off-spec polymer (in many cases equivalent to the minimization of the transition time). The third problem is the *load change problem* which can also be considered as a disturbance for quality control.

A large number of publications dealing with optimization and control of polymerization processes can be found in the literature (see e.g. Embirucu *et al.* (1996), Congalidis and Richards (1998) for a general review). The quality control problem is very frequently described, and in most cases model predictive control (MPC) technology is proposed for the quality controller (e.g. Ogunnaike (1994), Mutha *et al.* (1997), Prasad *et al.* (2002), Na and Rhee (2002), Young *et al.* (2002)). Despite the large number of recent articles dealing with the various aspects of polymerization reactor control most of these publications are from a relatively small number of active academic groups. Given the highly competitive and proprietary nature of commercial polymerization manufacturing technologies, it is also not surprising that contributions from industrial practitioners is rather limited (Congalidis and Richards, 1998). A small number of industrial applications exist and are published, but these are mainly concentrated on poly-olefine processes (e.g. McAuley and MacGregor (1991), Bhm *et al.* (1992), Kiparissides *et al.* (1997), Dittmar and Martin (1997), Seki *et al.* (1994)) where the above issues are nearly solved or not so relevant. Furthermore, off-line dynamic optimization problems have been formulated and solved for polymer grade transitions. Even though off-line optimization is routinely performed, its integration into the operation has been almost non-existent. Several reasons for this fact can be identified:

- The end-user might face the effect of a *combinatorial explosion*: Trajectories for all possible combinations of desired grades need to be pre-optimized and being held on shelf for all possible scenarios.

- For many processes, the *initial state* at the beginning of the transition is unknown: It might be estimated using state estimation techniques thus increasing the complexity of the application. Additionally, since the start of the trajectory generally is not only one nominal operating point, this also adds a potentially unlimited number of possible scenarios to be pre-optimized.

- The dynamic optimization is based on a process model with uncertain *model accuracy*. It is not clear in advance whether the model is sufficiently accurate to apply the pre-optimized trajectories without an additional feedback via a quality controller.

There have been significant advances in the sensor technologies for reliable measurements (**cite a reference**) in polymerization processes. However, this has not been

exploited for optimal operation in daily production using real-time optimization. Two major measurement-based approaches are classified as:

1. *Process model approach:* Here, measurements are used on-line to correct the current state of the process and re-estimate key model parameters. The controls are updated subsequently by a repetitive on-line solution of an optimization problem that utilizes a dynamic process model. It is referred to as *single level dynamic real-time optimization (D-RTO)*; its structure is identical to nonlinear model predictive control (NMPC) with output feedback. Its basic schematic is shown in Figure 1. For large-scale industrial applications, the D-RTO problem

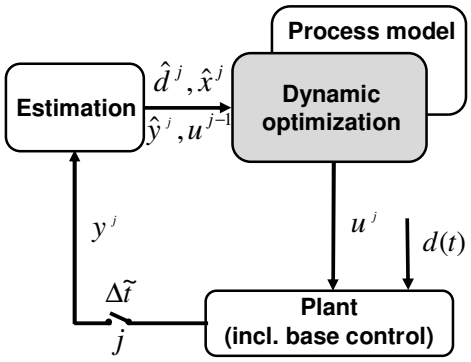


Figure 1: Single level D-RTO using process model

   is computationally expensive to solve. Due to the large computational requirements larger sampling intervals are demanded which may not be acceptable due to uncertainty. On the other hand, the current solution may not be qualitatively different from the previous one. Due to the complexity of D-RTO its acceptance in industry is limited.

2. *Solution model approach:* A conceptually different approach where, measurements are used to directly update the controls using a parameterized solution model that has been obtained from off-line optimization using a nominal dynamic process model (see Section 3).

This is a simplified control strategy for implementing the optimal solution and its uncertainty-invariant structure. The second approach is considered for application to a large industrial polymerization process involving grade transitions. The focus of the paper is on emphasizing the economical benefits rather than the classical control aspects of disturbance and noise rejection when using the solution model-based approach for a class of uncertainty leading to invariant solution model.

The paper is organized as follows: In Section 2 basics of the general dynamic optimization problem and its solution are presented. The solution model-based NCO tracking approach is introduced in Section 3. The industrial polymerization process is introduced in Section 4 along with the optimal grade change formulation and its numerical solution at the nominal conditions. This is followed by a characterization of the optimal solution in Section 5. The proposed solution model and NCO tracking

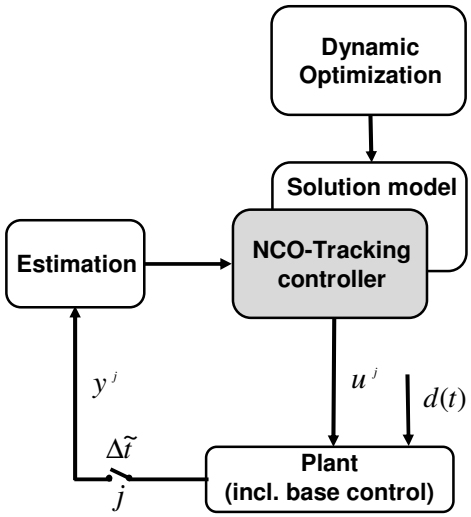


Figure 2: NCO tracking controller using solution model

results for different uncertainty realizations are presented in Section 6. The paper is finished with concluding remarks.

2 Preliminaries

2.1 Problem formulation and numerical solution

We consider the following terminal-cost dynamic optimization problem

$$\min_{\boldsymbol{u}(t),t_f} \Phi(\boldsymbol{x}(t_f),t_f) \tag{P1}$$

$$\begin{aligned} \text{s.t.} \quad & \dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u})\,, \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_0\,, && (1)\\ & \boldsymbol{0} \geq \boldsymbol{h}(\boldsymbol{x},\boldsymbol{u}), \quad t \in [t_0,t_f]\,, && (2)\\ & \boldsymbol{0} \geq \boldsymbol{e}(\boldsymbol{x}(t_f))\,, && (3) \end{aligned}$$

where $\boldsymbol{x}(t) \in \mathbb{R}^{n_x}$ denotes the vector of state variables with initial conditions $\boldsymbol{x}_0$. The process model (1) is formulated as the smooth vector function $\boldsymbol{f}$. The time-dependent control variables $\boldsymbol{u}(t) \in \mathbb{R}^{n_u}$ and possibly the final time are the decision variables for optimization. Furthermore, there are path constraints $\boldsymbol{h}$ on the states and control variables (2) and endpoint constraints $\boldsymbol{e}$ on the state variables (3).

There are various solution techniques available for dynamic optimization problems of the form (P1) (Binder *et al.*, 2001). In this work, we use the sequential or single-shooting approach, a direct method that solves the problem by transcribing into a nonlinear programming problem (NLP) through time-parameterization of the control variables $\boldsymbol{u}(t)$. We employ the software tool DyOS (Schlegel *et al.*, 2004) for this purpose.

For the parametrization of the control profile $u_i(t)$, piecewise-polynomial approximations (e.g. piecewise-constant or piecewise-linear) are often applied. The profiles for the state variables $\boldsymbol{x}(t)$ are obtained by forward numerical integration of the model (1) for a given input. With the discretization parameters $\hat{\boldsymbol{u}}$ as degrees of freedom (DOF), problem (P1) can be reformulated and solved as the NLP

$$\min_{\hat{\boldsymbol{u}}, t_f} \Phi(\boldsymbol{x}(\hat{\boldsymbol{u}}, t_f), t_f) \tag{P2}$$

$$\text{s.t.} \quad 0 \geq \hat{\boldsymbol{h}}(\boldsymbol{x}(\hat{\boldsymbol{u}}), \hat{\boldsymbol{u}}, t_i), \quad \forall\, t_i \in \Delta\,, \tag{4}$$

$$0 \geq \boldsymbol{e}(\boldsymbol{x}(\hat{\boldsymbol{u}}, t_f))\,, \tag{5}$$

with the path constraints being evaluated at the discrete time points contained in Δ.

2.2 Necessary conditions of optimality (NCO)

By employing Pontryagin's Minimum Principle (Bryson and Ho, 1975), problem (P1) can be reformulated with the *Hamiltonian* function $H(t)$ as

$$\min_{\boldsymbol{u}(t), t_f} \; H(t) = \boldsymbol{\lambda}^T \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}) + \boldsymbol{\mu}^T \boldsymbol{h}(\boldsymbol{x}, \boldsymbol{u}) \tag{P3}$$

$$\text{s.t.} \quad \dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u})\,, \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_0\,, \tag{6}$$

$$\dot{\boldsymbol{\lambda}}^T = -\frac{\partial H}{\partial \boldsymbol{x}}\,,\; \boldsymbol{\lambda}^T(t_f) = \left(\frac{\partial \Phi}{\partial \boldsymbol{x}} + \boldsymbol{\nu}^T \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{x}} \right)\Bigg|_{t_f}\,, \tag{7}$$

$$0 = \boldsymbol{\mu}^T \boldsymbol{h}(\boldsymbol{x}, \boldsymbol{u})\,, \tag{8}$$

$$0 = \boldsymbol{\nu}^T \boldsymbol{e}(\boldsymbol{x}(t_f))\,. \tag{9}$$

Here, $\boldsymbol{\lambda}(t) \neq \boldsymbol{0}$ denotes the adjoint variables, $\boldsymbol{\mu}(t) \geq \boldsymbol{0}$ and $\boldsymbol{\nu} \geq \boldsymbol{0}$ the Lagrange multipliers for the path and terminal constraints, respectively. The complementarity conditions (8)-(9) indicate that a Lagrange multiplier is positive if the corresponding constraint is active and zero otherwise.

An optimal solution of problem (P3) fulfills the necessary conditions of optimality:

$$\frac{\partial H(t)}{\partial \boldsymbol{u}} = \boldsymbol{\lambda}^T \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{u}} + \boldsymbol{\mu}^T \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{u}} = \boldsymbol{0}\,, \tag{10}$$

If a free final time is allowed, an additional transversality condition has to be also satisfied:

$$H(t_f) = \left(\boldsymbol{\lambda}^T \boldsymbol{f} + \boldsymbol{\mu}^T \boldsymbol{h}\right)\Big|_{t_f} = -\left.\frac{\partial \Phi}{\partial t}\right|_{t_f} \tag{11}$$

3 NCO tracking using a solution model

The NCO tracking adjusts the manipulated variables by means of a decentralized control system in order to track the NCO in face of uncertainty. This way, an almost optimal operation is implemented via feedback without the need for solving a dynamic optimization problem in real time. The real challenge lies in the fact that four different objectives (i.e. equations. (8)-(11)) are involved in achieving optimality. These path and terminal objectives are linked to active contraints (equations. (8), (9)) and to sensitivities (equations. (10), (11)). Hence, it becomes important to appropriately parameterize the inputs using time functions and scalars, and assign them to the different objectives. This assignment, which corresponds to choosing the *solution model*, is a way of looking at the NCO through the inputs.

The generation of a solution model includes two main steps (Srinivasan and Bonvin, 2004):

- *Input dissection:* Based on the effect of uncertainty, this step determines the fixed and free parts of the inputs. In some of the intervals, the inputs are independent of the prevailing uncertainty, e.g. in intervals where the inputs are at their bounds, and thus can be applied in an open-loop fashion. The corresponding input elements can be considered fixed in the solution model. In other intervals, the inputs are affected by uncertainty and need to be adjusted for optimality. All the input elements affected by uncertainty constitute the *free variables* of the optimization problem.

- *Linking the input free variables to the NCO:* The next step is to provide an unambiguous link between the free variables and the NCO. The active path constraints fix certain time functions and the active terminal constraints certain scalar parameters or time functions. The remaining degrees of freedom are used to meet the path and terminal sensitivities. Note that the pairing is not always unique. An important assumption here is that the set of active constraints is correctly determined and does not vary with uncertainty. Fortunately, this restrictive assumption can often be relaxed (Srinivasan and Bonvin, 2004).

Once the solution model has been postulated, it provides the basis for adapting the free variables using appropriate measurements. However, the solution model does not specify whether a controller needs to be implemented on-line or in a run-to-run fashion. On-line implementation requires reliable on-line measurements of the parts of the NCO used in the particular controller. In most of the applications, measurements of the constrained variables are available on-line. When on-line measurements of certain NCO parts are not available (e.g. sensitivities and terminal constraints), a model is used to predict them. Otherwise, a run-to-run implementation becomes necessary.

4 Case study example: Industrial polymerization process

This problem considers a real industrial polymerization process. The problem has been introduced by Bayer AG as a test case during the research project-INCOOP (Kadam *et al.*, 2003). Due to confidentiality reasons, only those details of process can be presented here which are published in the article by Dünnebier *et al.* (2004).

4.1 Process description

The flowsheet of this large-scale continuous polymerization process is shown in Figure 3. The exothermic polymerization process involving multiple reactions takes place in a continuously stirred tank reactor (CSTR) equipped with an evaporative cooling system. The reactor is operated at an open-loop unstable operating point corresponding to a medium level conversion. The reactor is followed by a separation unit for separating the polymer from unreacted monomer and solvent. They are recycled back to the reactor via a buffer tank. The polymer melt is further processed in downstream processing and blending units for the finished product properties. These are defined by the polymer viscosity and polymer content in the reactor which are in turn related to the molecular weight and conversion.

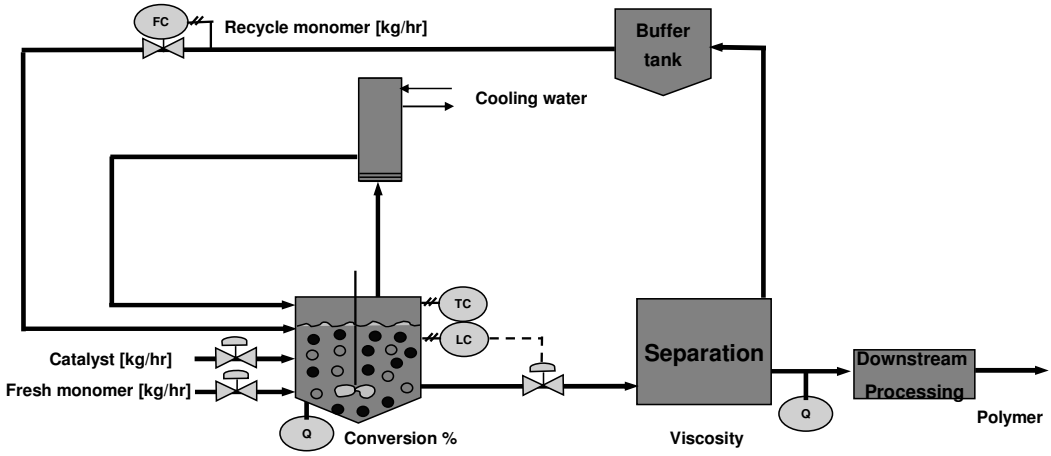


Figure 3: Simplified process flowsheet

4.2 Measurements

As in most quality control problems, the availability of reliable quality measurements is crucial for a successful implementation of the advanced process control. For a certain class of polymerization problems, the polymer quality (e.g. viscosity) can be observed from other measurements (e.g. concentrations) using a model. Therefore, control algorithms often rely on some kind of a soft sensor (such as neural network) instead of an online viscosity measurement. However, for this process, the polymer viscosity

is not observable from other online measurements. The following measurements are assumed to be available in the process:

- flowrates of recycle f_{RM} and fresh monomers f_{inM},
- flowrate of reactor outlet f_{rout},
- reactor temperature T_r and holdup V_R,
- buffer tank holdup V_{RT},
- solvent concentration sc,
- reactor conversion fg,
- polymer viscosity mw.

4.3 Process model

A rigorous reactor model including an extensive scheme of reaction kinetics is available from previous design and operation studies. The reactor and buffer tank are modelled in detail while the separation unit and condenser are simplified significantly using process insights. The reactor is modelled as a continuous stirred tank reactor (CSTR) with mass and energy balance and complex polymerization kinetics for all components involved. The separator is modelled as a static splitter. The condenser model is a grey box model, comprising static mass balances combined with a second order linear dynamic model identified from the process data. The reaction kinetics result in an open-loop unstable temperature dynamics (runaway reaction) at the nominal operating point. To prevent any temperature disturbance causing a quench down to the low temperature steady-state corresponding to low conversion or runaway up to the high temperature corresponding to high conversion, a feedback control scheme for the reactor temperature is required. Therefor, a stabilizing PID type controller for the reactor temperature is implemented in the model. The reactor holdup is maintained using a proportional control that manipulates the reactor outlet flowrate. The model is implemented in the dynamic simulation software gPROMS (gPROMS, 2002). The dynamic process model is significantly large with 200 differential and 2500 algebraic equations.

4.4 Optimal grade transition problem formulation

The same polymerization process is used to produce different grades of the polymer. Therefore, frequent grade changes are routinely performed in this process. An optimal change of the polymer grade is considered in this study. The task is to perform a change of the polymer grade A of the molecular weight of 0.727 ± 0.014 to grade B of the molecular weight of 1.027 ± 0.027 in a minimum time. During the transition operational constraints are enforced on the following quantities ($\boldsymbol{h}$):

- reactor outlet flowrate f_{rout},

- buffer tank holdup V_{RT},
- reactor conversion fg,
- polymer molecular weight mw,
- reactor temperature T_r,
- reactor solvent concentration sc.

Additionally, there are endpoint constraints on the reactor conversion fg and the polymer molecular weight mw (corresponding to the grade B specification), which are more strict than those enforced on these variables during the transition. There are three control variables $\boldsymbol{u}$ available, which are also shown in Figure 3: the flowrates of the fresh monomer f_{inM} and the catalyst f_{inC} feed streams as well as the flow rate of the recycle monomer f_{RM} stream. Even during the transition, the reactor holdup is maintained constant by manipulating the reactor outlet flowrate. Due to safety considerations and the lack of ideal mixing in the reactor, fast changes in the catalyst flowrate are not allowed in the plant.

The objective of the optimal grade change operation is to quickly change from the steady-state operating point producing grade A to the final steady state producing grade B while producing the least possible off-spec polymer. The overall objective function of the dynamic optimization problem can be mathematically formulated as the following:

$$\min_{\boldsymbol{u},t_{ss}} \Phi := \int_{t_0}^{t_{ss}} c_{mw}(mw(t) - 1.027)^2 + c_{fg}(fg(t) - 1.0)^2 dt \tag{12}$$

The final time t_{ss} is a degree of freedom in the optimization problem. Constant or time-variant weight factors c_{mw} and c_{fg} are used to penalize deviation in the polymer quality variables, molecular weight (mw) and reactor conversion (fg), from their grade B specifications during the transition. If the time-variant flowrate of the product stream is used as weighting factors, the objective function would correspond to minimization of the off-spec. polymer. A typical profile of the objective function defined above is depicted in Figure (4). As the objective function involving the amount of off-spec production is monotonic in this case, it is equivalent to the minimization of transition time (t_f) to change the polymer quality variables to the specifications of grade B. Furthermore, the objective function profile is almost constant after the grade B specifications are reached and the process is being stabilized to a steady-state.

The overall objective function is therefore a combination of two goals: 1) to minimize the transition time t_f and 2) to move subsequently the process to a steady-state corresponding to grade B while producing on-spec polymer. Hence the overall optimization problem is decomposed into an economical optimization problem:

$$\min_{\boldsymbol{u},t_f} \Phi_e := t_f, \tag{P$_\mathrm{e}$}$$

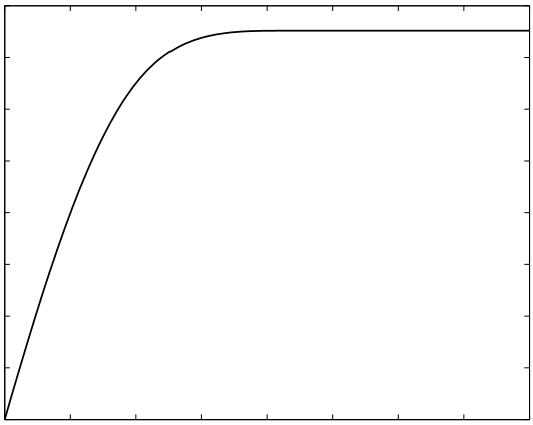


Figure 4: A typical profile of the objective function Φ

$$\begin{aligned} \text{s. t.} \qquad \boldsymbol{h}(t) &\leq 0, \\ \bar{mw} &\leq mw(t_f), \\ \bar{fg} &\leq fg(t_f), \end{aligned}$$

and a control problem:

$$\min_{\boldsymbol{u}} \Phi_c := \int_{t_f}^{t_{ss}} c_{mw}(mw(t) - 1.027)^2 + c_{fg}(fg(t) - 1.0)^2 dt + \dot{\boldsymbol{x}}(t_{ss})^T P \dot{\boldsymbol{x}}(t_{ss}), \quad (\mathrm{P_c})$$

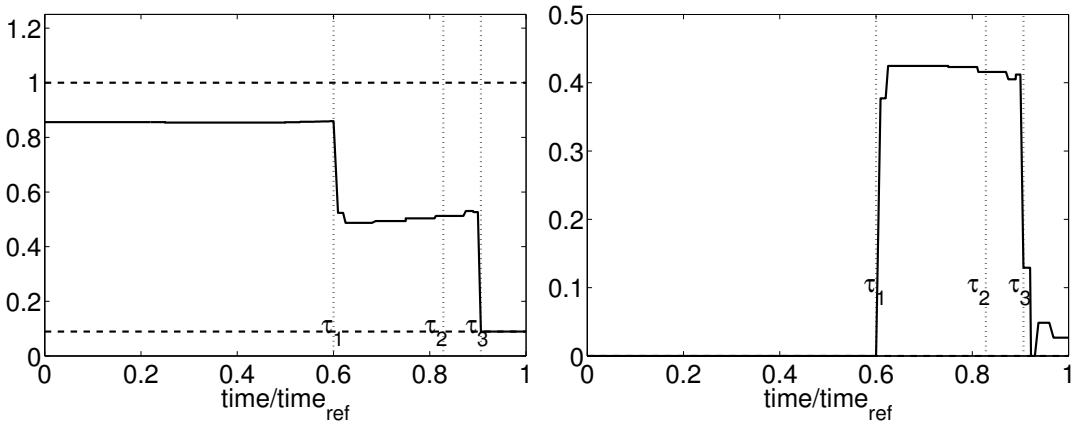
$$\text{s. t.} \quad \boldsymbol{h}(t) \leq 0.$$

In the control objective $\dot{\boldsymbol{x}}$ denote the state variable derivatives which are penalized by the matrix $\boldsymbol{P}$ to take the process to a steady state. The control time horizon $(t_{ss} - t_f)$ is fixed. In the above problem formulations, $\boldsymbol{h}$ are the operational path constraints explained before. As the objective functions and the endpoint constraint variables of the economical optimization problem $\mathrm{P_e}$ are monotonic, the decomposition is mathematically justified. Due to different objectives, the two Problems $\mathrm{P_e}$ and $\mathrm{P_c}$ can be treated separately. In this paper, the economical optimal grade change problem is considered. Problem $\mathrm{P_c}$ is a classic polymer production rate and quality control problem solved for grade B specifications after the the transition is realized. Furthermore, for this process, a load change (50% to 100% to 50%) problem which is similar to problem $\mathrm{P_c}$ is successfully solved in the article by Dünnebier *et al.* (2004).

4.5 Nominal optimal solution

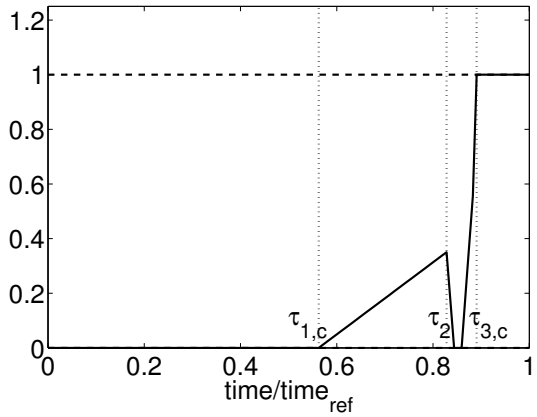
The optimal grade change problem $\mathrm{P_e}$ is solved using the dynamic optimizer DyOS (DyOS, 2002) which employs the single-shooting method for the solution of dynamic optimization problem. To find an accurate optimal solution with an identifiable structure, the wavelet-based adaptive refinement method proposed by Schlegel *et al.* (2004) is applied. For algorithmic details, the reader is referred to the aforementioned publication. The three control profiles (f_{inM}, f_{RM} and f_{inC}) are time-parameterized as

piecewise constant functions on the adaptively refined time grid for each control. The optimal solutions[2] are shown in Figure 5.



(a) Fresh monomer flowrate f_{inM}

(b) Recycled monomer flowrate f_{RM}

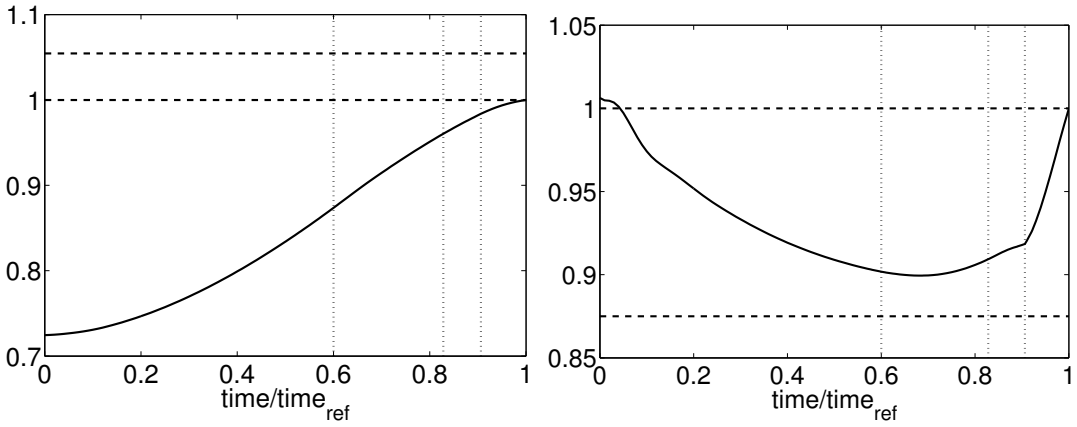


(c) Fresh catalyst flowrate f_{inC}

Figure 5: Optimal profiles of the control variables

The optimal profiles of the polymer quality variables and the path constraints are shown in Figure 6 and 7. As the grade change is a planned one, the optimization problem is solved off-line. Sufficiently accurate optimal solution is calculated using adaptively refined parametrization grids for each control. The computational time required to solve the problem is significantly smaller than the transition time. A numerical analysis of the solution techniques applied for this problem is out of the focus of the paper. For details in this regard, the reader is referred to (Kadam, 2003). A distinct yet complex structure is present in the optimal solution and the the path and end-point constraints. This is discussed in detail in the following section.

[2]For confidentiality reasons, both axes in all the solution plots and any numbers related to this problem are scaled.



(a) Viscosity mw (b) Conversion fg

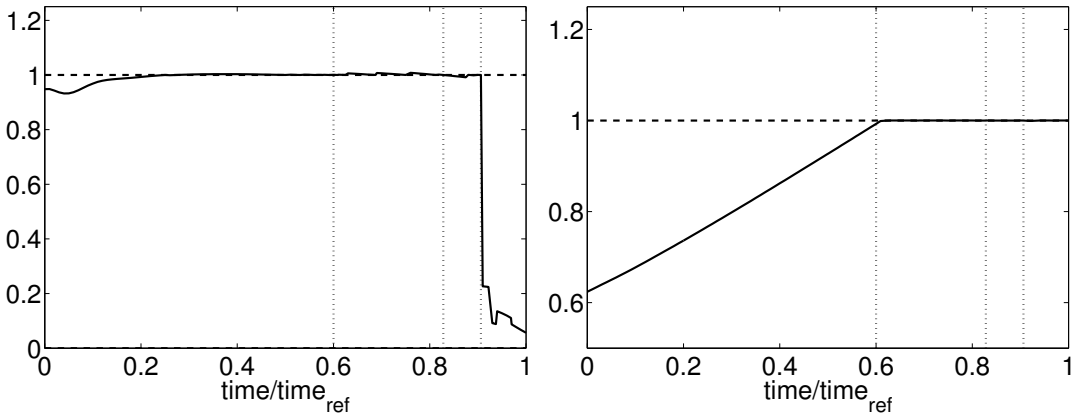
Figure 6: Optimal profiles of the polymer quality variables

5 Characterization of the optimal solution

The optimal solution is analyzed for insights into the grade change operation, which are used for implementing the solution under uncertainty. The reactor holdup is kept constant using a controller that manipulates the reactor outlet flowrate. Due to this it can be noted that the total monomer (fresh + recycled) flowrate is equal to the reactor output flowrate. Furthermore, the reactor temperature set-point is fixed at a value corresponding to grade B. And, the catalyst flowrate is manipulated to effect a change in the polymer molecular weight. Furthermore, the residence time (V_r/f_{rout}) of the reactor affects the reactor conversion and in turn the polymer molecular weight. Using this physical insight the optimal solution is characterized next.

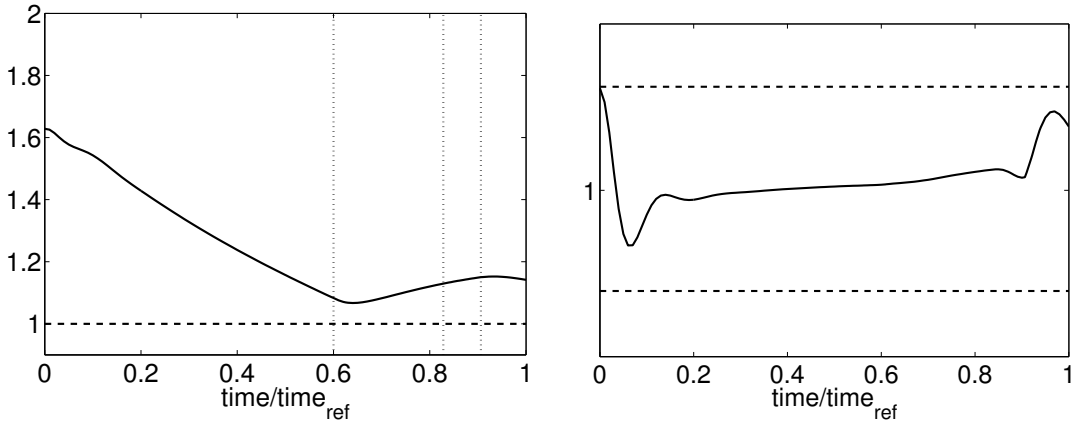
The optimal solution of f_{inM} and f_{RM} consists of three arcs while that of f_{inC} has four. On each arc, the controls are labelled as {*path, sensitivity* or *bound (min or max)*}- seeking controls. This separation of controls is done by *visually* analyzing the control and active path constraint profiles. The identified structure of the solution described by the active controls and path constraints is given in Table 1. An automatic structure detection along with the calculation of an optimal solution is recently studied by Schlegel and Marquardt (2004).
The interpretation of the solution on each arc is as follows:

1. *Arc 1:* The path constraint on the reactor output flowrate f_{rout} is kept active at its upper bound by manipulating flowrate of the fresh monomer, while the other two controls, flowrates of the recycled monomer f_{RM} and fresh catalyst f_{inC}, are kept at their respective lower bounds. The f_{inM} is referred to as path constraint-seeking while both f_{RM} and f_{inC} are labelled minimum bounded. Essentially, the fresh monomer is fed into the reactor while the reactor content is removed as quickly as possible. As the reactor holdup is maintained constant, the reactor output flowrate is increased in response to the increased flowrate of the fresh monomer. As the residence time is reduced not all monomers can be reacted, which are recycled back through the buffer tank. The reactor sol-



(a) Reactor outlet flowrate f_{rout}

(b) Buffer tank holdup V_{RT}



(c) Reactor solvent concentration sc

(d) Reactor temperature T_r

Figure 7: Optimal profiles of the path constraint variables

vent concentration and conversion reduce but do not hit their respective lower bounds.

2. *Arc 2:* As the recycled monomers are temporarily stored in the buffer tank, its hold up V_{RT} continually increases and hits the upper bound at $t = \tau_1$. On arc 2 starting at τ_1, V_{RT} is maintained at the upper bound by manipulating f_{RM}. This results into an increase in the total monomer flowrate to the reactor. To maintain the reactor holdup, f_{inM} is simultaneously reduced and manipulated to keep f_{rout} at the upper bound. Note that the two coupled controls are simultaneously manipulated to keep the two constraints active and hence are labelled on this arc path constraint-seeking. Approximately at the same switching time ($\tau_{1,C}$), f_{inC} is changed linearly till the end ($t = \tau_2$) of arc 2. As the sensitivity the two active path constraints with respect to f_{inC} is very small, the control is referred to as sensitivity-seeking.

3. *Arc 3:* At $t = \tau_2$, f_{inC} is switched to its lower bounds, hence called as minimum bounded control. The other f_{inM} and f_{RM} are path constraint-seeking controls

Table 1: Structure of the optimal solution of problem P_e

Arc k	Interval $[\tau_{k-1}, \tau_k]$	$f_{inM}(t)$	$f_{RM}(t)$	$f_{inC}(t)$	$f_{rout}(t)$	$V_{RT}(t)$	$mw(t_f)$	$fg(t_f)$
1	$[0,\ 0.6]$	Path	Min	Min	Active			
2	$[\tau_1 = 0.6,\ 0.83]$	Path	Path	Sens	Active	Active		
3	$[\tau_2 = 0.83,\ 0.91]$	Path	Path	Min	Active	Active		
4	$[\tau_3 = 0.91,\ 1.0]$	Min	Path	Max		Active		
	$t_f = 1.0$						Active	Active

as they are manipulated to keep f_{rout} and V_{RT} at their bounds. This sudden change in the catalyst flowrate is to give a sudden push to the polymer molecular weight towards the target value of grade B.

4. *Arc 4:* This arc starts at $t = \tau_3$ by switching f_{inM} to its lower bound. Due this the path constraint on f_{rout} is deactivated. f_{inM} is labelled minimum bounded control. The active constraint on V_{RT} is maintained by manipulating the path-constraint seeking control f_{RM}. This is done to increase the reactor residence time to further increase the polymer molecular weight mw and conversion fg. Approximately at the same time $\tau_{3,C}$, f_{inC} is switched to its upper bound resulting in an increase in mw. By this time, fg and sc are significantly reduced from their initial values but do not violate their constraints. As shown in Figure 7, fg starts increasing almost linearly on arc 4 and eventually reaches its lower end-point constraint target value $\bar{fg}$ at the end of the transition at $t = t_f$. mw also reaches its lower end-point constraint $\bar{mw}$ at the same time, i.e. both the end-point constraints are active at t_f. Note that, during this arc, the slope of mw profile is continuously reduced, but it does not become zero, hence not risking a reduction in the molecular weight away from $\bar{mw}$. The slope should be properly monitored and controlled during this kind of grade transition operation. This insight will be used during an implementation (in simulation) of the dynamic optimization solution in the subsequent section.

The characterization of the optimal solution provides a very useful insight. It is emphasized that this is possible only due to the accurate optimal solution of this complex dynamic optimization problem and the fairly good prediction model for dynamic optimization. In the absence of this, an adequate physical insight and knowledge about close to optimal process operation may allow this kind of characterization of the dynamic operation. However, this is rarely available in an industrial scenario. Especially, in the presence of uncertainty, a characterization for optimal operation is difficult to corroborate from the process date and knowledge. The characterization of the optimal solution is exploited for a possible implementation using only the available measurements.

6 Implementation of the optimal solution using solution models

The optimal grade transition problem is solved for a given initial state of the process operated at steady-state for polymer grade A. In reality, the initial state comprising all the differential variables of the model is infrequently estimated from the available measurements using the process model. Various kinds uncertainties are present in this polymerization process. As a representative of uncertainty for the simulation studies, we have chosen the effect of a set of unknown components accumulating in the reactor due to the recycle stream on the polymerization reaction. When operating the process for a long time, concentration of unknown components increases while the solvent concentration reduces significantly. Note that the solvent is not continuously added to the process, but the recycled monomer is purged and replaced by fresh solvent if its concentration reaches a certain threshold. Due to this operational scenario, the initial state of the process along with the initial solvent concentration can be different from the nominal for a realization of the grade A to B transition. These condition are simulated using the model by manipulating one parameter in the model and changing the reactor temperature set-point. Furthermore, due to uncertainty, an update of the nominal optimal solutions is necessary before their implementation.

In this work, a radically different approach is considered for an update and implementation of the dynamic optimization solution in the presence of uncertainty. As explained in Section 3, a solution model derived from the nominal optimal solution is employed for the implementation for optimal transition. Repetitive solutions of the large dynamic optimization problem using the process model is avoided by exploiting the nominal solution and measurements. The following requirements for such an approach are fulfilled for this process.

- *Invariant optimal solution structure:* For verification, re-optimizations are performed for different realizations of the uncertainty explained before. It is observed that, for this class of uncertainty, the structure of the optimal solution - the number, type and sequence of arcs - does not vary. Hence, the structure of the solution is invariant. In reality this assumption has to be qualified with respect all kinds of uncertainty. However, the assumption has been found to be qualified for the operation scenarios at hand. Moreover, it is observed that some of the nominally in-active path constraints become active and vice-versa for realization of certain values of the uncertainty. This has to be correctly handled during an implementation, which is discussed in the next section.

- *Availability of measurements or estimates:* On-line reliable measurements of the polymer quality variables and other constraint variables are available (see Section 4.2). In case measurements are not available, a multi-rate EKF estimator has been implemented (Dünnebier *et al.*, 2004) for estimating the required variables. Therefore, for the simulation studies in this paper it is assumed that the measurements are available.

- *Adequate fidelity of the optimal solution:* A rigorous process model is used for

calculating the nominal optimal solutions presented in Section 4.5. It is found to be valid for a large range of load and polymer grades. Fidelity of process model is described by accuracy of prediction of the sensitivities of key variables with respect to controls. On each arc of the optimal solution, the normalized sensitivities (the direction $\frac{\Delta y}{\Delta u}$) are in line with those given by the plant-replacement model. The fidelity of this optimal solution is therefore adequate.

6.1 Solution model

Due to complexity of the polymerization process and operational uncertainty, the process model can not be maintained and updated frequently. The accurate optimal solution of the grade A to grade B transition problem are directly used and updated using only measurements. In sequel, the process model is used for simulation studies as a plant-replacement only.

The solution model in Figure 8 is derived by considering the characterization of the optimal solution presented in Section 5. Before presenting the solution model, a simplification of the optimal solution for implementation is done. Note that a solution model is just an approximation of the optimal solution under uncertainty. The optimal profile of catalyst consists of four arcs: minimum bounded, linearly increasing sensitivity-seeking, minimum bounded and max bounded arc. The second and fourth arc are present to feed fresh catalyst into the reactor. Without sacrificing much on the optimality (the transition time), the profile is approximated with a constant sensitivity-seeking arc of value f_{inC}^0 followed by an arc of constant value $f_{inC}^{\tau_3}$ starting at $t = \tau_3$. The transition time using this profile for the catalyst flowrate is only slightly increased. Now the optimal solution consists of two arcs for f_{inM}, three for f_{RM} and two for f_{inC}. The switching times τ_1, τ_3 and the transition time t_f are also the degrees of freedom (DOF) of optimization under uncertainty. In the derived solution model in Figure 8, the time-variant arcs and time-invariant switching times are linked to certain parts of the necessary conditions of optimality of problem $\mathrm{P_e}$.

1. *Fixed arcs:* Flowrate of the fresh monomer f_{inM} is fixed at $f_{inM}^{\tau_3}$ in arc 3 ($\tau_3 \leq t \leq t_f$). Flowrate of the recycled monomer f_{RM} is fixed at its lower bound in arc 1 ($0 \leq t \leq \tau_1$). And, the remaining control f_{inC} is fixed in arc 1 ($0 \leq t \leq \tau_1$) at f_{inC}^0 and in arc 3 ($\tau_3 \leq t \leq t_f$) at its upper bound $f_{inC}^{\tau_3}$. As the process is stabilized to a steady-state for grade B after the grade transition, final value of the monomer flowrate $f_{inM}^{\tau_3}$ and the catalyst flowrate $f_{inC}^{\tau_3}$ are fixed according to the target production rate. Furthermore, f_{inC}^0 as the initial value of f_{inC} is adapted on a run-to-run basis such that a positive slope in the profile of mw is maintained throughout the transition. This ensures that mw continually changed towards the grade B specification.

2. *Path constraint-seeking arcs:* During the operation, all path constraints need to be respected. Therefore, the controls f_{inM} and f_{RM} are adapted on-line using measurements of the constraint variables that become active. In the nominal optimal solution, only the constraints on f_{rout} and V_{RT} are active. However, the remaining path constraint variables may become active for a certain value of the

initial state. Therefore, all the quantities are *monitored* for activation of their respective constraints. An RGA analysis is done to separate the two controls f_{inM} and f_{RM} for linking them separately to constraint variables using SISO controllers. The designed superstructure of controllers $(C_1, \ldots, C_5)$ along with their triggering mechanism is shown in Figure 8. f_{inM} is linked to the reactor output flowrate f_{rout} to maintain at its setpoint f_{routSP}. In case the reactor conversion fg reaches its upper or lower bound, f_{routSP} is accordingly changed from its otherwise fixed value of the upper bound f^U_{rout}. Furthermore, f_{RM} is linked to the nominally active constraint on the buffer tank holdup V_{RT}. The solvent concentration sc is reduced during the transition according to the process dynamics. If sc reaches its lower bound, f_{RM} is adapted using measurement of sc to maintain at the bound. It has been observed that the constraints on V_{RT} and sc cannot be active at the same time, thus avoiding violation of either of the constraints.

Note that measurement of a constrain quantity is necessarily used for adaptation of the controls only when it is on its constraint. The designed input-output pairings are implemented using controllers in the gPROMS model used as plant replacement. To demonstrate benefits of the NCO tracking using solution model, simple PID type controllers are employed in this study for the control of purpose. The use of advanced controllers for tracking the active constraints may be employed for better tracking performance (Dünnebier *et al.*, 2004). For the employed PID type controllers, the nominal solution of the controls is used as the feed-forward part, which is found to be satisfactory from the controller performance point of view.

3. *End-point constraint-seeking DOF:* In the nominal optimal solution, both end-point constraints of mw and fg are active at the end (t_f) of transition. According to the optimality condition, t_f is determined as the time when both end-point constraints become feasible $(\bar{mw} \leq mw(t_f)$ and $\bar{fg} \leq fg(t_f))$. The unlinked switching time τ_3 as the starting time of arc 3 is related to one of the end-point constraints for making it feasible at the end. As explained in the characterization of the optimal solution, the profile of fg increases almost linearly in arc 3 after the active constraint on f_{rout} is deactivated at τ_3. Furthermore, slope of the profile of mw is continually decreasing. Therefore, it is likely that mw moves away from its target value of grade B during arc 3. Due to these facts, τ_3 is adapted on-line such that both mw and fg are simultaneously made feasible at the end. A process data-based empirical model

$$mw^{pred}(t) = f(mw(t), \dot{mw}(t), (fg(t) - \bar{fg})) \tag{13}$$

is identified for predicting $mw^{pred}(t)$ if τ_3 is assigned as the current time and the controls are adapted as given in step (1). The adaptation law for τ_3 is as follows:

$$\tau_3 = t, \text{ such that } mw^{pred}(t) \geq \bar{mw}. \tag{14}$$

Note that the model uses measurements of $mw(t)$, its slope $\dot{mw}(t)$ and $fg(t)$. In the fixed time $t_f - \tau_3$, both mw and fg move in the end-point feasible region.

Parameters of empirical model (13) are adapted using measurements from the past grade transition operation.

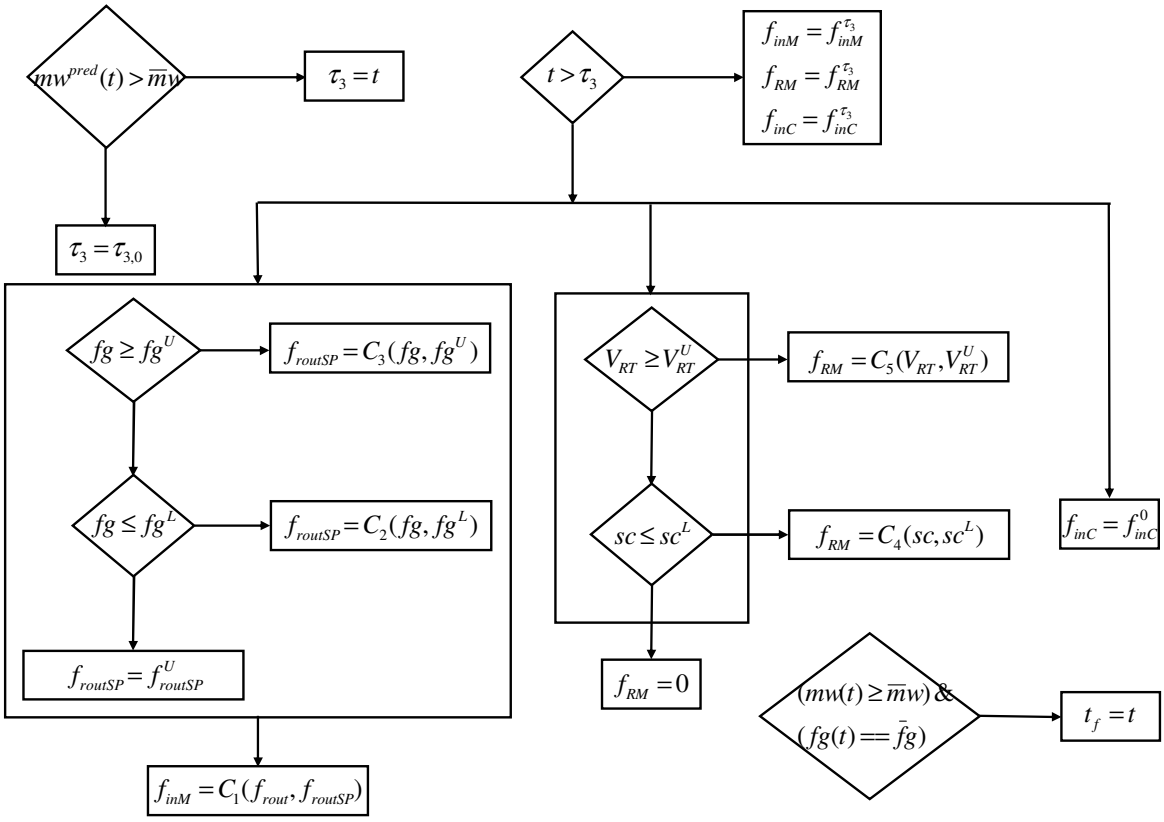


Figure 8: Solution model and trigger mechanism of the optimal solution

The process schematic with the proposed controller superstructure is shown in Figure 9. The derived solution model is based directly on the optimization problem formulation. Therefore, simulation profiles of the combined solution and process model are an approximation of the optimal solution under uncertainty. As simple controllers with non-optimal tuning parameters are employed, the realization is sub-optimal, yet feasible with respect to all constraints. The use of solution model for enforcing the necessary conditions of optimality (NCO) seems a simplified strategy for an industrial application point of view.

6.2 NCO tracking results

The proposed hybrid control structure for realizing optimal grade change operation in the presence of uncertainty is implemented in the plant replacement model. The performance of this control strategy is tested first for the nominal initial state of the process. Note that other process disturbances such as measurement noise are not considered in this study to mainly focus on the aspect of optimization. The tracking controllers and the empirical model (13) are tuned for the nominal case.

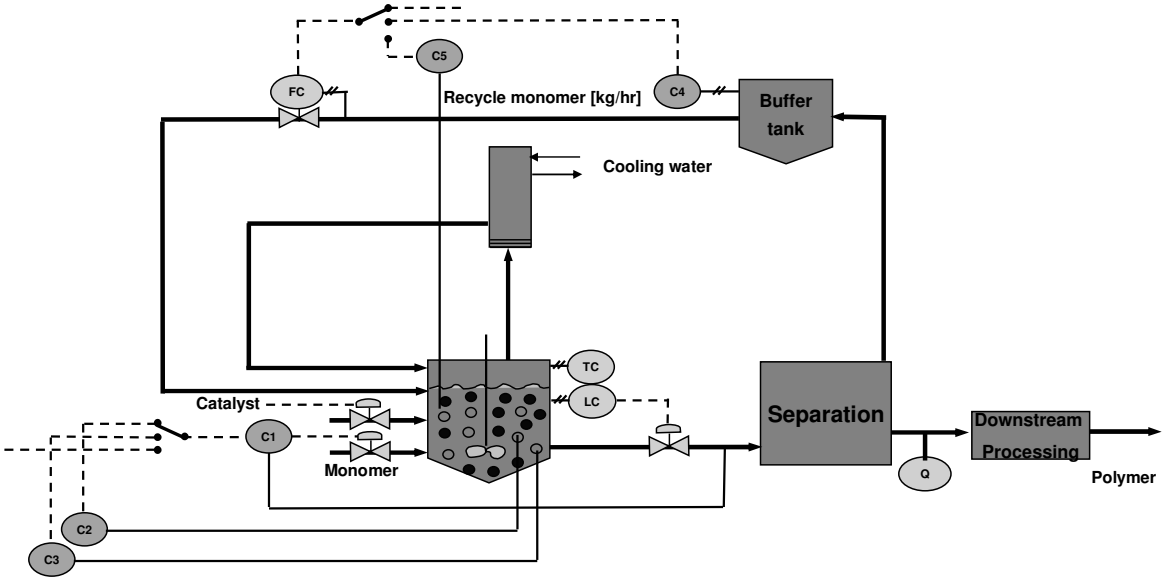
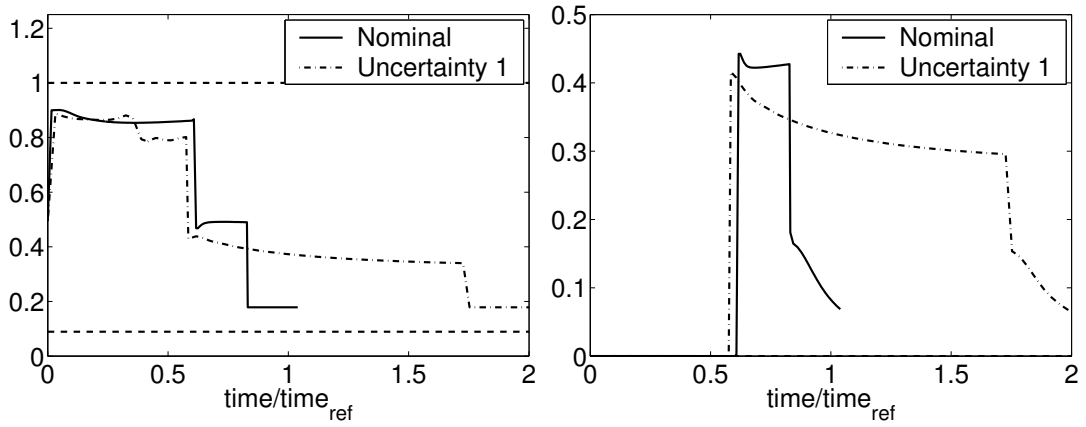


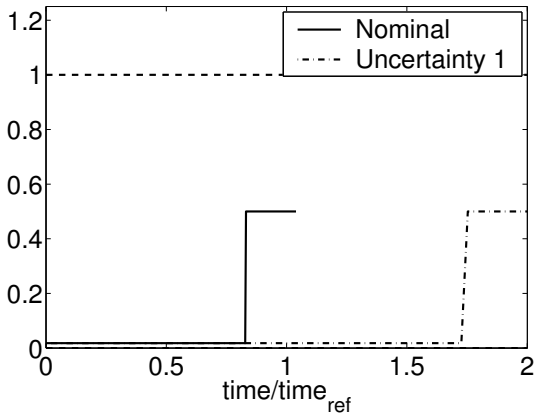
Figure 9: Simplified process flowsheet with the NCO tracking controllers and triggers

Only measurements of the quantities required in the solution model are used for the implementation. The simulated NCO-tracking profiles are depicted in Figures 10–12 as bold lines. The control profiles are adapted by the controllers which are triggered according to the proposed solution model in Figure 8. The profiles of the controls and constraint variables are almost the same as the nominal optimal profiles. The switching time τ_3 and the catalyst flowrate after that $f_{inC}^{\tau_3}$ are adapted according to the empirical model such that mw and fg are simultaneously feasible at the end. The approximation of the optimal catalyst flowrate for implementation increases the transition time by only 0.8%.

For the nominal case the loss in optimality using the solution model is expected to be minimal. The same NCO-tracking controllers and their tuning parameters are used for the grade transition with two different initial states of the process (uncertainty 1 and 2). At these steady-states of grade A, different from the nominal concentration of the solvent and accumulated unknown components are considered. The simulated NCO-tracking profiles for uncertainty 1 are depicted by dash-dotted lines in Figures 10–12. The transition time is larger than that for the nominal case. Furthermore, all the path and end-point constraints are feasible. The nominally inactive constraint on fg becomes active for this case (Figure 11(b)). When the constraint on fg becomes active, the reactor outlet flowrate is automatically manipulated as shown in Figure 12(a). Note the negative slope in the mw profile in arc 3 during which fg increases linearly. The empirical model (13) uses measurements of the slope to predict sufficiently accurate mw at the end. A more accurate empirical model based on the original process model and past measurements can improve its prediction quality and hence the economical performance. An accurate adaptation of τ_3 and $f_{inC}^{\tau_3}$ is crucial in fulfilling the end-point constraints on mw and fg. During this arc, a neighboring extremal controller (Kadam and Marquardt, 2004) for manipulating f_{inC} or setpoint



(a) Fresh monomer flowrate f_{inM} (b) Recycled monomer flowrate f_{RM}



(c) Fresh catalyst flowrate f_{inC}

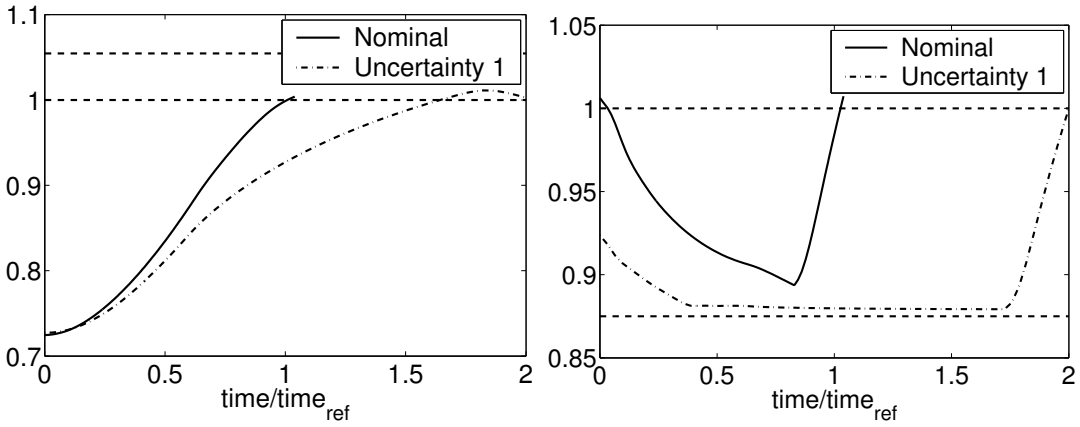
Figure 10: NCO-tracking profiles of the control variables

of the reactor temperature controller can be employed for a tighter quality control. To avoid zero reactor outlet flowrate in the longer than optimal arc 3, f_{inM} is not switched to its lower bound but to the value corresponding to the target steady-state load for grade B. After the transition, the process is anyway going to be stabilized at the 100% load. The grade transition problem is re-optimized using the uncertain initial states in the process model as known values. The grade transition time using the solution model and the re-optimized controls (ideal case) are given in Table 2.

Table 2: Grade transition time using different optimization strategies

Case	Solution model	Re-optimization (Ideal)	Optimality loss %
Nominal	1.008	1.0	0.8
Uncertainty 1	2.03	1.81	12.15
Uncertainty 2	0.938	0.915	2.51

The optimality loss given as the increase in transition time from the ideal case is quite small under different uncertainty scenarios. The NCO-tracking controllers can



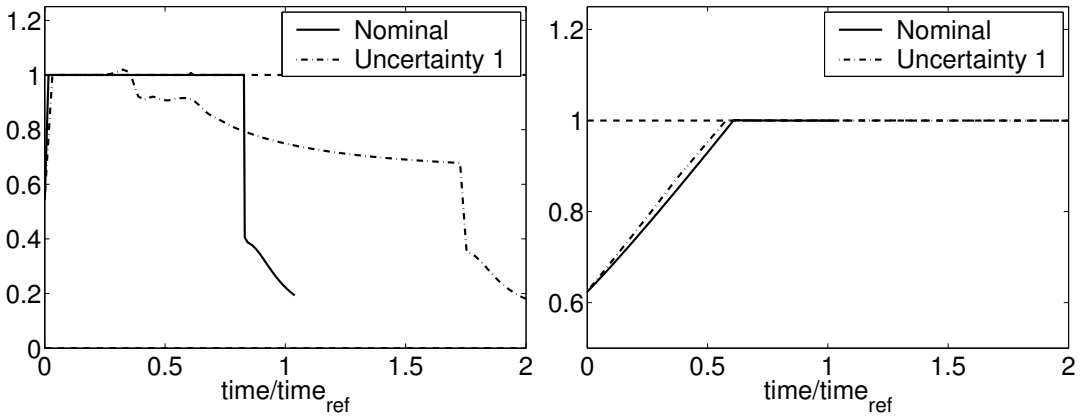
(a) Viscosity mw (b) Conversion fg

Figure 11: NCO-tracking profiles of the polymer quality variables

be re-tuned online for each case for better performance. Furthermore, the operation is feasible with respect to the path constraints as well as the end-point constraints. With these results, it is demonstrated that a simplified hybrid control strategy using a solution model and measurements can realize the complex grade transition solution. It is only fair to mention that the derivation of the solution model still requires an accurate optimal solution for the nominal case and some physical insight into the process. However, the simulated economical benefits in the terms of reduction in the transition time and hence the off-spec polymer production is quite significant than the conventional approach practice in the plant. For limited grade transition scenarios, nominal optimal solutions can be calculated off-line and realized using solution model-based NCO-tracking controllers. Therefore, the problem of process model maintenance and update for this kind of control strategy is simplified to a certain extent. However, reliable measurements or model-based estimates of certain problem variables are required at different times during the operation for an applicability of this type of strategy.

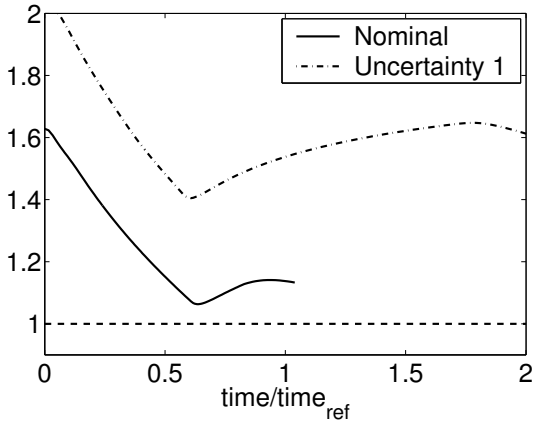
7 Conclusion

In this paper, we have shown the application of the NCO-tracking approach proposed by Srinivasan *et al.* (2003) to a simulated industrial polymerization process. The NCO are tracked using a solution model and measurements to realize a feasible and almost optimal operation under uncertainty. The solution model consists of state-event triggered controllers sequenced according to the structure of the optimal solution. A planned grade transition optimization problem is considered for an industrial polymerization process. The nominal optimal solution of three control variables exhibits a complex structure involving many active path constraints and end-point constraints. The off-line computed optimal solution shows significant reduction in the grade transition time and off-spec polymer production when compared to the conventional strategies used by operators. However, an implementation of the optimal solution in the presence of uncertainty associated with polymerization processes is

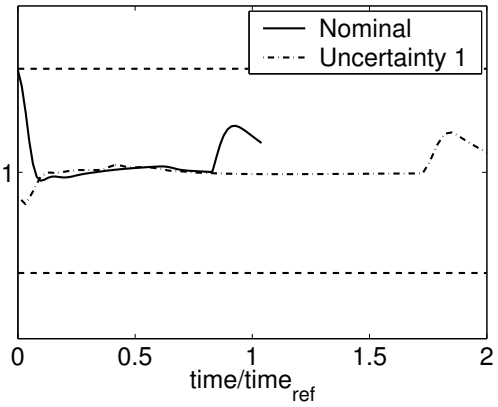


(a) Reactor outlet flowrate f_{rout}

(b) Buffer tank holdup V_{RT}



(c) Reactor solvent concentration sc



(d) Reactor temperature T_r

Figure 12: NCO-tracking profiles of the path constraint variables

difficult. In this study, the uncertainty of unknown initial state of the process with different solvent concentration is considered. A solution model is derived from the nominal optimal solution. An approach of superstructure of controllers is considered to handle activation of nominally inactive path constraints. Simple PID type controllers are used to realize the solution model. For different uncertainty scenarios, the simulation of the solution model shows that a feasible operation is possible. Furthermore, the loss of optimality is low. The NCO-tracking controllers using the solution model and measurements adapt the controls automatically such that all constraints are satisfied. The control strategy to enforce the structure of the optimal solution under uncertainty is quite simple and robust for implementation in industry. Though a process model is not employed for on-line implementation, reliable measurements of quality and constraint variables are necessary. Moreover, a constant solution structure is assumed for this approach for a given type of uncertainty during operation. To handle various problems in operation, the approach should be integrated in a general framework of dynamic optimization and control that uses both a fundamental process model and a solution model.

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