OPTIMISATION OF GRADE TRANSITIONS IN AN INDUSTRIAL GAS-PHASE OLEFIN POLYMERIZATION FLUIDIZED BED REACTOR VIA NCO TRACKING

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Abstract: Gas-phase olefin polymerization fluidized-bed reactors are complex processes that are characterized by large time constants and slow transitions. Optimal grade changes can be computed off-line on the basis of a detailed process model and applied to the process in an open-loop mode. However, the presence of uncertainties in the form of process-model mismatch and disturbances make this approach clearly non-optimal. Fortunately, measurements can be used to improve the situation; this can be done either *explicitly* via process model refinement and repeated optimisation, or *implicitly* via direct input adjustment. This work considers the optimisation of grade-transition changes by enforcing on-line the necessary conditions of optimality (NCO tracking) using available measurements. The key steps are the generation of an adjustable model of the optimal solution and its adaptation using appropriate measurements or estimates of the controlled variables. A realistic simulation process model is employed to compare the performance of NCO tracking to that obtained via the open-loop application of nominal optimal trajectories. *Copyright © 2005 IFAC*

Keywords: Adaptation technique, on-line optimal control, optimality conditions, polymerization, polyolefin production, grade transition.

1. INTRODUCTION

Operating a steady-state continuous polymerization process in an optimal way satisfying certain economic criteria is a common task for the process operator. However, when a grade transition is involved, the task complexity tremendously increases due to the inherently dynamic character of the transient process operation. Experience-based recipes are commonly inferior to optimal control policies, thus, depriving the full exploitation of plant's potential. Consequently, model-based optimisation

techniques, using advanced mathematical programming, are employed instead. The economic importance of product quality optimisation has motivated extensive research efforts aiming at the development of dynamic optimal control policies for different polymerization processes. Thus, a great number of studies on open-loop optimal control of polymer quality (e.g., number- and weight-average molecular weights, polydispersity index, copolymer composition, molecular weight distribution, etc.) have been reported for batch and semi-batch polymerization reactors (Cawthon and Knabel, 1989; Choi and Butala, 1991; Crowley and Choi, 1997). Moreover, in a number of published reports, the actual application of the calculated optimal control policies to laboratory and industrial polymerization reactors has been demonstrated. To account for process-model mismatch and unknown process

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disturbances, the off-line calculated optimal control policies need to be continuously updated via on-line parameter and state estimation and/or corrective feedback control (Kim and Choi, 1991; Kozub and MacGregor, 1992; McAuley and MacGregor, 1993; Kiparissides et al., 1994; Ogunnaike, 1994; Kiparissides et al., 1996 and 2002).

The dynamic optimisation literature is largely concerned with the off-line calculation of optimal control policies based on the availability of a detailed process model. On the other hand, there are only a limited number of studies regarding the use of process measurements to account for parameter uncertainty (e.g., model-process mismatch, disturbances etc.) prevailing in an industrial application. The aim of this study is to present a computational framework that uses available measurements to update directly the optimal inputs (instead of the time-varying model parameters) via the tracking of the necessary conditions of optimality (NCO). The NCO-tracking technique (Srinivasan et al., 2002a,b) is applied to a simulated olefin polymerization plant that captures the dynamic features of a real industrial gas-phase olefin polymerization fluidized bed reactor.

2. OPTIMISATION VIA NCO TRACKING

2.1 Measurement-based optimisation

In the face of growing competition, process optimisation has recently received considerable attention because it represents a natural choice for reducing production costs, improving product quality, meeting safety requirements and environmental regulations. The standard *nominal optimisation* approach is based on the numerical calculation of the optimal solution, given a model of the process. However, in practical situations, an accurate process model can rarely be found with affordable man-month effort. In the presence of state and control constraints, modelling errors and disturbances may lead to either infeasible or non-optimal operation.

In this work, the main idea is to employ a *measurement-based optimisation* approach where the available measurements are used to compensate for uncertainty. In this context, the dynamic optimal control policies can be calculated and updated on-line via the satisfaction of the necessary conditions of optimality (NCO). Note that the structure of the on-line NCO-tracking strategy is derived from the off-line numerical optimisation of a nominal model.

2.2 Generation of the NCO-tracking model

For the generation of a NCO-tracking model for a *dynamic process*, it is important to note that the solution of a constrained terminal-time dynamic optimisation problem is typically discontinuous and consists of various arcs and intervals. Hence, the NCO-tracking model will include both path and terminal objectives, since there are conditions that have to be met during the operation while others need to be satisfied at the final time. Furthermore, optimality implies keeping certain constraints active and certain sensitivities at zero. Thus, the enforcement of the NCO for a dynamic optimisation problem corresponds to satisfaction of four sets of conditions (i.e., a constraint part and a sensitivity one active during the plant operation and at the final time) using appropriate measurements.

Hence, it becomes important to appropriately parameterize the control inputs using time functions and scalars and assign them to the different tasks. This assignment, which corresponds to choosing the *solution model*, is a way of looking at the NCO through the inputs. Thus the calculation of a NCO-tracking solution model includes two steps:

(i) **Input dissection:** This is based on the effect of uncertainty on the optimal solution and determination of fixed and free input variables. The generation of a solution model typically starts with the numerical optimisation of a nominal process model (possibly incorrect). The resulting optimal solution is analysed for several uncertainty realizations. For some of the time intervals, the inputs are (or are assumed to be) independent of the prevailing uncertainty, (e.g., intervals where the inputs are at their bounds). Therefore, they can be applied in an open-loop fashion. These input elements can thus be considered fixed in the NCO-tracking solution model. In other intervals, the inputs are affected by uncertainty and need to be adjusted for optimality. All the elements affected by uncertainty constitute the free variables of the optimisation problem. The number and sequence of input arcs as well as the parameterization of the inputs in various arcs form the core issue in input dissection.

(ii) **Linking the input free variables to the NCO.** The next step is to provide an unambiguous link between the free input variables and the NCO. The active path constraints are linked with certain time functions and the active terminal constraints with certain scalar parameters or time functions. The remaining degrees of freedom are used to meet the path and terminal sensitivities. 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.

2.3 Formulation of adaptation laws

Once the solution model is formulated. it provides the basis for adaptation of the various free parts of the inputs using appropriate measurements. Depending upon the availability of the measurements, these updating laws can be implemented either on-line or on a run-to-run basis. Run-to-run adaptation has two main drawbacks: (i) it does not compensate for variations within a run since

only disturbances that are correlated over several runs can be rejected, and (ii) it requires multiple runs to be optimal. Thus, if possible, it is preferable to do most of the adaptation on-line.

However, the required information on the path sensitivities and terminal objectives is typically not available during the run. This necessitates information regarding the future, a task that requires a reliable process model, which was assumed to be unavailable in this study. This implies that full adaptation cannot, in general, be accomplished within a single run. However, the emphasis is to make judicious approximations and formulate strategies to get as much as possible within a single run.

3. OLEFIN POLYMERIZATION PROCESS

3.1 Process description

Gas-phase catalytic olefin polymerization processes are well known for their product versatility, which is a powerful economic and technical advantage. This polymer property versatility is achieved through appropriate manipulations of the process operating conditions. Therefore, the optimal control and operation of such a process is of crucial importance.

In a catalytic gas-phase olefin polymerization FBR (see Figure 1), catalyst particles are continuously fed into the reactor, at a point above the gas distributor, and react with the incoming fluidizing reaction medium (e.g., monomers, H_2, N_2) to produce a broad distribution of polymer particles. A good dispersion of catalyst throughout the reaction zone is essential to prevent the formation of localized hot spots. Usually, the catalyst is continuously fed into the bed carried by an inert gas (e.g., nitrogen) that provides a means for reactor pressure control. Chatzidoukas et al. (2003) developed a detailed mathematical model to study the dynamic operation and optimisation of an industrial olefin polymerization FBR. The process operating conditions and all the kinetic and model parameters are given in the same publication.
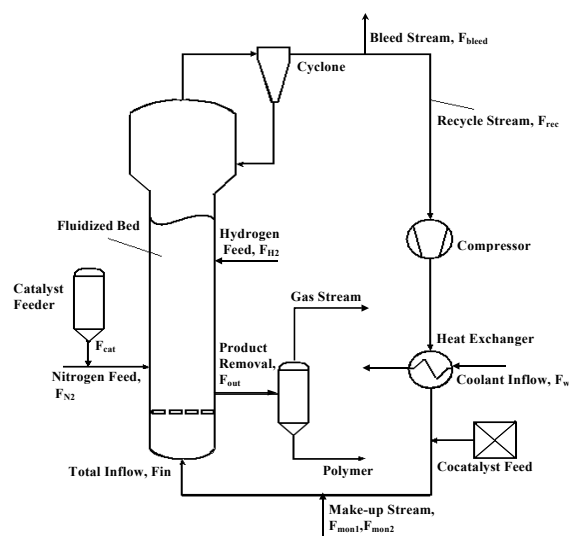

Fig 1. Gas-phase olefin copolymerization FBR unit.

3.2 The grade transition problem

It is often the case that the polymer produced during a grade transition does not meet both the initial and the final product specifications. It is therefore important to consider how this transition can be implemented with as little economic penalty as possible. A mathematical formulation of the optimisation problem is crucial for the calculation of optimal solution for a grade transition problem. It should fully capture both the optimisation objectives and the plant constraints. Note that incorporation of the designer intuition and knowledge of the process are necessary to constrain the process variables to lie within the plant capabilities. Commonly, the optimal solution to a grade transition problem is based on the minimization of a suitable objective function defined in terms of the changeover time, product quality specifications, process safety constraints and the amount of off-spec polymer, using dynamic optimisation numerical techniques.

In general, the objective function is a measure of process profitability. However, in order to avoid purely economic terms (e.g., hypothetical scenarios in terms of time-fluctuated market demands for different polymer grades and the specification of production times for each grade), an implicit objective function is employed in terms of polymer melt index and density. These polymer quality indexes are indicative of the end-use polymer properties (e.g., stiffness, transparency, hardness, etc.) as well as the rheological and processability characteristics of polyolefins. Hence, a polymer is assumed to be within product specifications if its MI and ρ values are within some acceptable desired ranges. In the present study, an integral quadratic objective function was defined in terms of MI and ρ deviations from their desired final values.

3.3 Formulation of the optimisation problem

The two major economic objectives (i.e., minimization of the off-spec product amount and minimization of the transition time) that reflect the process profitability during a grade transition, are implicitly accounted for in the following objective function definition:

$$\min_{\text{Ratio}, F_{H_2}, h_{sp}, R_{p,sp}, t_f} \mathbf{J} = \int_{t_o}^{t_f} \left\{ \left(\frac{MI(t) - MI_f}{MI_0 - MI_f} \right)^2 + \left(\frac{\rho(t) - \rho_f}{\rho_0 - \rho_f} \right)^2 \right\} dt$$

Minimization of the above objective function is subject to a system of **DAEs**, describing the process dynamics, and to the following constraints on the process and quality variables:

$$\rho_{LB} \leq \rho_f \leq \rho_{UB}$$

$$MI_{LB} \leq MI_f \leq MI_{UB}$$

$$T_{LB} \leq T_f \leq T_{UB}$$

$$P_{LB} \leq P_f \leq P_{UB}$$

$$h_{LB} \leq h_f \leq h_{UB}$$

$$R_{p,LB} \leq R_{p,f} \leq R_{p,UB}$$

$$\dot{MI}_{LB} \leq \dot{MI}_f \leq \dot{MI}_{UB}$$

The subscripts 0 and f denote the corresponding values of the "polymer quality" variables at the start and the final time of a grade transition, respectively. The subscripts LB and UB denote the lower (LB) and upper bounds (UB) of the respective process variables (i.e., density (ρ), melt index (MI), temperature (T), pressure (P), bed level (h), production rate (R_p) and time derivative of melt index ($\dot{MI}$)). Notice that the time derivative of MI, representing the slowest dynamic variable of the process, is additionally constrained to guarantee the attainment of a steady-state at the end of a transition.

In the present study, the time optimal control policy for the transition from grade A to grade B was determined for a gas-phase catalytic ethylene-1-butene copolymerization FBR. The selected product specifications for grades A and B as well as the corresponding operating conditions at steady state, are reported in Table 1. As can be seen, the transition from grade A to B results in a polyolefin having a higher melt index MI, and a lower density ρ. Four manipulated variables (i.e., the comonomer/ monomer ratio in the make-up stream, R, the hydrogen flow rate, F_{H_2}, the set points of the bed level and production rate, h_{sp}, $R_{p,sp}$) and the final time were treated as free variables.

A dynamic optimisation method based on control vector parameterization (i.e., gPROMS/gOPT, Process Systems Enterprise Ltd.) was selected to calculate the optimal control transition policies. The control inputs were assumed to be piecewise constant and the time domain was discretised into 5 time intervals.

4. GRADE TRANSITION VIA NCO TRACKING

4.1 Optimisation under uncertainty

The developments described so far represent a nominal case where no uncertainties are considered. However, parametric uncertainties might appear because of the various assumptions and approximations made during model developments and/or the presence of unknown process disturbances. In practice, an accurate model that fully describes a real process can rarely be found. In a polyolefin plant, the major source of uncertainty is related to the catalyst activity and, therefore, the kinetics of all the stages of the polymerization mechanism. For example, the catalyst activity (e.g., the potential metal catalyst sites and their activity distribution) is a very common source of parametric uncertainty. Furthermore, even in the case that these parameters are accurately known (i.e., via lab-scale experimental measurements) their actual values might alter in an industrial reactor where the conditions are significantly different from those in the lab.

In this study, two types of uncertainty were considered resulting in two hypothetical operating scenarios of the polyolefin FBR that substantially differ from the so-called nominal case. In the first uncertainty scenario, it was assumed that the values of the kinetic rate constants for the chain-transfer to hydrogen reactions were inaccurate and, therefore, their actual values differed from the respective nominal ones (1st type of uncertainty):

$$K_{tH,1}^1 = K_{tH,2}^1 = 80\ \{\text{nominal value} = 88\}\,(\text{cm}^3/\text{mol/s})\ ;$$
$$K_{tH,1}^2 = K_{tH,2}^2 = 350\ \{\text{nominal value} = 370\}\,(\text{cm}^3/\text{mol/s})$$

In the second uncertainty scenario, it was assumed that the fractions of the potential catalyst sites f_i in the fresh catalyst feed deviated from their nominal values in addition to the uncertainty regarding the values of the kinetic parameters mentioned above (2nd type of uncertainty):

$$f_1 = f_2 = 0.5\ \{\text{nominal values: } f_1 = 0.6 \text{ and } f_2 = 0.4\}$$

4.2 Model of the optimal solution

For the transition from grade A (i.e., lower melt-index and higher density) to grade B (i.e., higher melt-index and lower density), measurements-based adjustments of the hydrogen feed rate and monomer ratio profiles were considered. The bed level and production set points did not change drastically with uncertainty and so were kept at the values obtained from the nominal optimisation. For the identification of NCO-tracking solution models for the hydrogen feed rate and the monomer ratio profiles the following steps were applied:

1. **Input dissection:** The optimal solution was dissected into 3 intervals: (i) In the first interval, the hydrogen feed rate and the monomer ratio were at their upper bounds to increase the polymer melt-index and decrease the density. (ii) In the second interval, the hydrogen feed rate was set to its lower bound in order to "brake" the increase of the polymer melt-index. (iii) In the third interval, the hydrogen feed rate and the monomer ratio were kept at time-varying "optimized" values to achieve the specifications for melt-index and density.

2. **Parameterization:** The two inputs were parameterized using five parameters: (a) two

Table 1. Operating conditions and product specifications for grades A and B

Operating Conditions	Grade A	Grade B
h_{sp} (m)	6.0	6.0
T_{sp} (K)	360	360
P_{sp} (bar)	21	21
$R_{p,sp}$ (g/s)	2390	2390
F_{bleed} (g/s)	0.1	0.1
F_{rec} (g/s)	$1.33\ 10^5$	$1.33\ 10^5$
Product specifications		
M_w (g/mol)	$3.8\ 10^5$	$2.9\ 10^5$
Φ_2	0.024	0.046
ρ (g/cm³)	0.9299 (±0.05%)	0.919 (±0.05%)
MI	0.01376 (±4%)	0.036 (±4%)

switching instants (t_1 and t_2), (b) a time-varying profile for each input in the third interval (i.e., $F^3_{H2}(t)$ for the hydrogen feed rate and $R^3(t)$ for the monomer ratio), and (c) the final time (t_f). The active terminal constraints correspond to the final desired values of the melt-index, density, and the derivative of melt-index.

3. **Linking input parameters with NCO:** The coupling of the optimal solution parameters with the necessary conditions of optimality was done next. Two of the three active terminal constraints (i.e., melt-index and density) were coupled with the levels of hydrogen feed rate and monomer ratio. The value of the final time, t_f, was linked with the satisfaction of the terminal constraints for the derivative of the melt-index (i.e., $-\varepsilon \leq \dot{MI}_f \leq \varepsilon$). The two switching times (t_1 and t_2) were treated as sensitivity-seeking parameters.

4.3 Formulation of adaptation laws

The model of the solution is given as follows:

$$F_{H_2} = \begin{cases} F_{H_2,max} & 0 \leq t < t_1 \\ F_{H_2,min} & t_1 \leq t < t_2 \\ F_{H_2}^{nom} + K_F(MI - MI_{f,des}, \rho - \rho_{f,des}) & t_2 \leq t < t_f \end{cases}$$

$$R = \begin{cases} R_{,max} & 0 \leq t < t_2 \\ R^{nom} + K_R(MI - MI_{f,des}, \rho - \rho_{f,des}) & t_2 \leq t < t_f \end{cases}$$

$$t_1 = t_1^{nom} + K_{t1}(H_2^{nom}(0) - H_2(0))$$

$$t_2 = t_2^{nom} + K_{t2}(\dot{MI}^{nom}(t_1) - \dot{MI}(t_1))$$

$$t_f = t \text{ s.t.} \|\dot{MI}\| = \dot{MI}_{min}$$

The switching times (t_1 and t_2) were determined using the neighboring extremal technique. Accordingly, the deviation between the actual and nominal initial hydrogen concentrations was employed to correct the value of t_1. Similarly, the deviation between the actual and nominal melt-index derivatives was used for the second switching time (t_2). In the third interval, the terminal constraints on melt-index and density were met using feedforward control action (derived from the nominal solution) together with a 2x2 multivariable PI controller that manipulated the hydrogen feed rate and the monomer ratio. Finally, the optimal value of t_f was determined via the satisfaction of the end-point constraints on the derivative of the melt index.

4.4 Simulation results

The optimization capabilities of the NCO-tracking solution were tested for the two uncertainty scenarios described in the previous section. In Table 2, the nominal, optimal and NCO-tracking values of the objective function and final transition time are reported for a transition from grade A to grade B. Note that the nominal results correspond to the off-line calculated hydrogen feed rate and monomer ratio optimal trajectories using erroneous values for the kinetic parameters and catalyst fractions. The ideal results correspond to the respective off-line calculated optimal trajectories with known parametric uncertainty, and the NCO-tracking results correspond to the respective optimal trajectories obtained on-line using the NCO-tracking solution. The dynamic evolution of the melt-index, density, hydrogen feed rate and monomer ratio are shown in Figures 2-5.

It can be seen that when the nominal solution is applied (i.e., without accounting for parameter uncertainty) the calculated transition time is nearly four times longer than that obtained by the optimal solution (i.e., accounting for parameter uncertainty). Note that the calculated nominal trajectories fail to bring the plant within the desired product specifications because the model does not account for parameter uncertainty. As a result, the feedback controllers need a significantly longer time to bring the process within the desired product specifications. On the other hand, NCO tracking provides a solution fairly close to the optimal one, calculated off-line for known parameter uncertainty. The superior performance of the NCO-tracking solution is partly due to the successful adaptation of the switching times (i.e., the addition of the required hydrogen amount) and to the combined feedforward/feedback control of the hydrogen feed rate and the monomer ratio during the third interval.
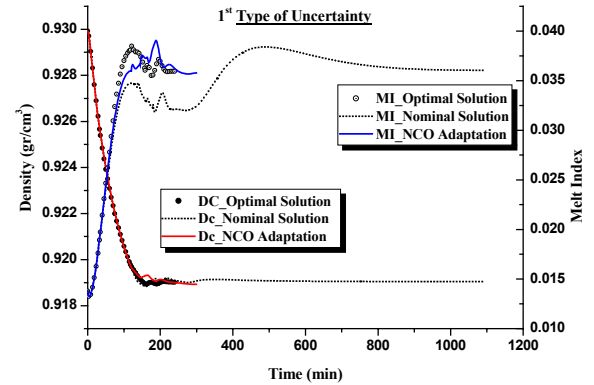

Fig. 2. Calculated density and MI profiles for the transition from grade A to B under parametric uncertainty (1st uncertainty scenario).

Table 2. Comparison of the calculated values of the objective function and final time for a transition from grade A to grade B

	Nominal Solution (Unknown Uncertainty)		Ideal Solution- (Known Uncertainty)		NCO Tracking Solution	
	Objective Function	**Time (min)**	**Objective Function**	**Time (min)**	**Objective Function**	**Time (min)**
1st Uncertainty Scenario	4.76038	1091.97	4.26592	240.36	4.3132	295.5
2nd Uncertainty Scenario	4.54711	1051.74	4.1593	272.4	4.17839	289.1

It is important to note that this improvement is obtained within a single run while run-to-run adaptation could be used to further improve the solution. Moreover, the NCO-tracking solution does not require knowledge of the model parameters.

5. CONCLUSIONS

In the present study, the NCO-tracking optimisation method has been applied to a simulation model of an industrial olefin polymerization FBR. The proposed strategy is based on available on-line measurements used to update the optimal solution in order to meet the NCO. The solution model, calculated off-line, is adapted to the real process via feedforward control and measurement-based feedback laws to force the plant to track the optimality conditions. Comparison of the process operation under the NCO tracking approach and under the off-line calculated nominal optimal solution indicated the major economic benefits gained through the application of the NCO-tracking policy.
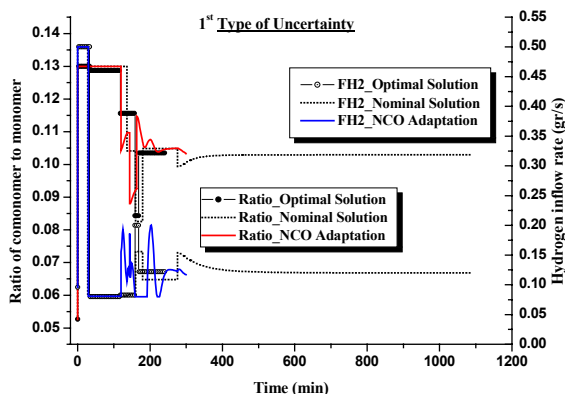

Fig 3. Time optimal control policies of the comonomer/monomer ratio and the hydrogen flow rate for the transition from grade A to B under parametric uncertainty (1st uncertainty scenario).
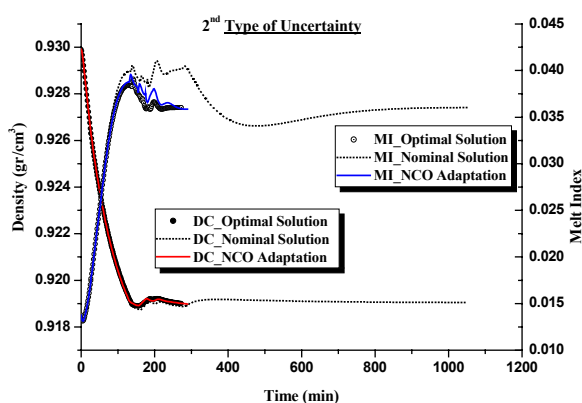

Fig 4. Calculated density and MI profiles for the transition from grade A to B under parametric uncertainty (2nd uncertainty scenario).

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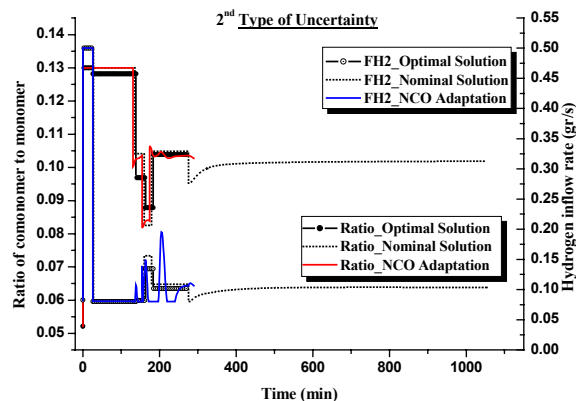
Fig 5. Time optimal control policies of the comonomer/monomer ratio and the hydrogen flow rate for the transition from grade A to B under parametric uncertainty (2nd uncertainty scenario).

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