RECONFIGURATION IN THE MODEL PREDICTIVE CONTROL OF NUMBERED-UP MODULAR FACILITIES

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Abstract

Modular production units are small-scale modules that are implemented into a working facility by numbering-up modules to achieve a desired throughput. While many supply chain studies have demonstrated the benefits of modular process designs, the potential operation and control benefits of a numbered-up system have not been as well studied. In this work, we analyze the possibility of reconfiguring modular connectivity in response to set point changes. In particular, the set point tracking performance for a system of three benchmark reactor modules is analyzed. Simulation results identify a breakpoint where for larger set point changes it is more beneficial to reconfigure from a parallel to hybrid configuration. Obtaining this knowledge through offline simulations is useful to keep the configuration and control action decisions separate and the optimal control problem tractable.

Keywords

Network reconfiguration, Modular manufacturing, Model predictive control.

Introduction

Over the past few years, global events such as a pandemic, war, climate change, and social unrest have made clear the fact that future infrastructure that supports human life, such as the production of critical chemicals such as fertilizers and fuels, must be sustainable. A promising approach to further enabling sustainable development, resource independence, and a modern circular economy is to implement distributed, rather than centralized, chemical supply chains. Distributed manufacturing can be broadly defined as utilizing large numbers of small-scale geographically scattered facilities, which is beneficial to reducing transportation costs for geographically distributed resource supply or product demand. A pivotal facilitating technology for distributed manufacturing is that of modular production units. These are small-scale, standardized units that can perform traditional or intensified chemical unit operations (Baldea et al., 2017; Shao and Zavala, 2020). Modular units can be constructed off-site at a centralized manufacturing site, transported to a chemical production facility, and quickly assembled together to a working plant. Due to their inherent small scale, they may also be disassembled and moved to other facilities as needed. Desired plant throughput is achieved by "numbering-up", or installing and connecting multiple copies of the same module type. Unlike traditional chemical facilities but analogous to trends in, for example, the manufacture of automobiles, favorable economics for modular systems are achieved via an economy of numbers, where building many units makes capital costs lower, rather than an economy of scale, where building larger units makes capital costs lower.

Recent research has explored and demonstrated the many possible benefits of distributed supply chains with modular production units. From an economic perspective, it has been demonstrated that such systems are well equipped

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to exploit spatiotemporal variability in, for example, the supply of critical feedstocks or the demand of the product made (Allman and Zhang, 2020). Additionally, it has been shown that increasing production capacity in a supply chain by building modular units can help to mitigate risk of sunk capital investment in cases where economic conditions such as future demand forecasts are uncertain (Shao et al. 2021). Practically speaking, distributed modular supply chains have shown to be promising in the production of ammonia (Palys et al. 2018), the upgrading of shale gas to higher value chemicals (Allen et al. 2019), and the processing of biomass waste into energy (Allman et al. 2021), to name a few examples.

Much of the recent process systems research on modular facilities has looked at supply chain level problems. However, for decisions made on the time scale of scheduling, real-time operation, and control, there exist several potential benefits (and challenges) that can occur when considering a numbered-up modular facility rather than a facility with a single scaled up process unit. In particular, we note that when operating a numbered up system, there exists the option of attempting to control each module individually, or only worrying about a system wide output, allowing for a disturbance in one module to be rejected by manipulating another module's input. Depending on which is chosen, symmetry may emerge in the underlying optimal control problem, which can make it challenging to find high quality solutions and requires a symmetry-breaking or dimensionality reduction approach. Finally, while it intuitively makes most sense to operate numbered-up modules in parallel, the opportunity exists to dynamically transition the module configuration to a series architecture, or any number of hybrid series/parallel architectures that may involve mixing together or splitting module output streams. The act of reconfiguration can potentially reject system disturbances more quickly, achieve lower costs in changing economic conditions, or allow for the production of different qualities of product. This work focuses on analyzing the potential for reconfiguration of modular connectivity in the control of a numbered-up modular system.

Modern chemical process control of complex systems is often performed using model predictive control (MPC), whereby an optimization problem is repeatedly solved in a moving horizon fashion in order to determine control actions. Typically, the resulting optimization problem formulation is a nonlinear program (NLP), which are commonly solved for this application using a fast local solver such as IPOPT (Biegler and Zavala, 2009). Introducing the action of reconfiguration to the optimal control problem adds integer variables (corresponding to the module connectivity), resulting in a mixed integer nonlinear program (MINLP) as the optimal control problem. Unfortunately, MINLPs are much more difficult to solve than NLPs and typically cannot return a solution of high quality in the time scale relevant for control decisions. As such, it is desirable to decouple the decisions of module configuration and process control by, for example, simulating system dynamics and control for different configurations offline and attempting to learn and understand which configurations work best for different values of the control problem parameters (i.e. set points, initial states, and feed conditions), such that the configuration can be seen as fixed in the optimal control problem.

This work provides an initial effort towards the above goal by studying the set point tracking of a modular system with benchmark reactor units when changing modular configuration. The remainder of the paper is structured as follows. The next section presents the optimal model predictive control problem considered in this work, with emphasis on how module configuration affects the underlying model. The following section provides additional detail on the various problem instances analyzed in this study. Then, we present the results of various set point tracking simulations and provide assessments of control performance when switching between configurations. Finally, we conclude by summarizing this work and suggesting some potential ideas for future development.

Problem Statement and Formulation

In this work, we aim to perform MPC on a numbered-up system of benchmark reactors whose dynamic model is adapted from Liu et al. (2009). In particular, each reactor can perform a series of first order reactions A→B→C, to convert a feed consisting of only A to the desired product B, with C as an undesirable side product. Our goal of control is to drive the final output mass fraction of B, x_B, to its set point, as well as to keep each individual module at a temperature set point. This is achieved by manipulating the flow of fresh feed to each module, as well as the heating rate to each module. Each reactor follows the standard assumptions of a continuously stirred tank reactor (CSTR). The formulation of the optimal MPC problem is as follows, with the notation for this problem presented in Table 1.

Table 1. Nomenclature for problem formulation

Symbol	Description
$\mathcal{I}$	Set of modular units
$\mathcal{I}_o$	Set of modular units connecting to output stream of the system
$\mathcal{T}$	Set of time points
$\mathcal{M}$	Set of species (reactants and products) in the system
w_x	Weighted parameters for mole fraction term in the objective function
w_T	Weighted parameters for temperature terms in the objective function
w_F	Weighted parameters for flow rate terms in the objective function

w_F	Weighted parameters for heat rate terms in the objective function
n_{ij}	Binary, 1 if there is a flow from modular unit i (output) to j (input)
$x_{b,sp}$	Set point of mole fraction of desired product B in final output
$T_{i,sp}$	Set point of temperature for modular unit i
N	Total number of modular units
k	Arrhenius pre-exponential factor
H	Enthalpy of reaction
V	Volume of the modular unit
E	Activation energy of reaction
ρ	Average density of the reactant-product mixture
c_P	Heat capacity of the reactant-product mixture
R_{gas}	Universal gas constant
F_{ijt}	Flow rate from modular unit i to j at time point t
F_{fit}	Flow rate of fresh feed to modular unit i at time point t
F_{iot}	Flow rate from modular unit i to final output at time point t
Q_{it}	Heating rate for modular unit i at time point t
T_{it}	Temperature of modular unit i at time point t
T_f	Temperature of feed
x_{imt}	Mole fraction of species m in modular unit i at time point t
x^*_{mt}	Mole fraction of species m in the final output at time point t

As is typical for model predictive control, the objective function is to minimize a weighted combination of discretized integral square error terms on the process outputs, and integral square control terms on the process inputs:

$$\sum_{t\in\mathcal{T}}(w_x\left(x^*_{bt}-x_{b,sp}\right)^2+\sum_{i\in\mathcal{J},j\in\mathcal{J},i\neq j}\left(w_T\left(T_{it}-T_{i,sp}\right)^2+w_F\left(F_{ijt}-F_{ij,t-1}\right)^2+w_Q\left(Q_{it}-Q_{i,t-1}\right)^2\right)) \quad (1)$$

The problem is constrained by the time-discretized dynamic model that describes material and energy balances in our benchmark modular reactor units. All of the following equations hold for all modules $i \in \mathcal{J}$ and all time points in the control horizon $t \in \mathcal{T}$, unless otherwise specified. First, consider the following material balances for species A in the each module:

$$x_{iA,t+1}=\Delta t\left(\frac{F_{fit}}{V}+\sum_{j\in\mathcal{J},i\neq j}n_{ji}\frac{F_{jit}x_{jAt}}{V}-\left(\sum_{j\in\mathcal{J},i\neq j}n_{ij}F_{ijt}+F_{iot}\right)\frac{x_{iAt}}{V}+f_1(T_{it},x_{iAt})\right)+x_{iAt} \quad (2)$$

Where the reaction term is:

$$f_1(T_{it},x_{iAt})=\ k_1\exp\left(\frac{-E_1}{R_{gas}T_{it}}\right)x_{iAt} \quad (3)$$

Note that the above mass balance is valid for any configuration, and which specific flow terms are considered for a specific configuration are determined by the binary parameter n_{ji}, which is one when the current configuration enables flow from module j to module i, and zero otherwise. For example, in a two module parallel configuration $n_{12}=0$, while in a series configuration, $n_{12}=1$. For the purpose of this study, values of these parameters are assumed to be fixed, which allows for a simpler implementation of the material balances once the configuration is known. Similarly, the material balance for species B in each module is:

$$x_{iB,t+1}=\Delta t\left(\sum_{j\in\mathcal{J},i\neq j}n_{ji}\frac{F_{jit}x_{jBt}}{V}-\left(\sum_{i\in\mathcal{J},j\in\mathcal{J},i\neq j}n_{ij}F_{ijt}+F_{iot}\right)\frac{x_{iBt}}{V}+f_1(T_{it},x_{iAt})-f_2(T_{it},x_{iBt})\right)+x_{iBt} \quad (4)$$

Where the second reaction term is:

$$f_2(T_{it},x_{iBt})=\ k_2\exp\left(\frac{-E_2}{R_{gas}T_{it}}\right)x_{iBt}, \quad (5)$$

An energy balance is used to derive the change in temperature over time:

$$T_{i,t+1}=\Delta t\left(\frac{F_{fit}T_f}{V}+\sum_{j\in\mathcal{J},i\neq j}n_{ji}\frac{F_{jit}T_{jt}}{V}-\left(\sum_{j\in\mathcal{J},i\neq j}n_{ij}F_{ijt}+F_{iot}\right)\frac{T_{it}}{V}+g_1(T_{it},x_{iAt})+g_2(T_{it},x_{iBt})+\frac{Q_{it}}{c_P\rho V}\right)+T_{it},\ \ \forall i\in\mathcal{J} \quad (6)$$

Where the reaction terms are:

$$g_1(T_{it},x_{iAt})=-\frac{H_1m}{c_P}k_1\exp\left(\frac{-E_1}{R_{gas}T_{it}}\right)x_{iAt} \quad (7)$$

$$g_2(T_{it},x_{iBt})=-\frac{H_2m}{c_P}k_2\exp\left(\frac{-E_2}{R_{gas}T_{it}}\right)x_{iBt} \quad (8)$$

Since one of the key assumptions of a CSTR is constant mass holdup in each reactor, we also define a steady state overall mass balance constraint:

$$F_{fit}+\sum_{j\in\mathcal{J},j\neq i}F_{jit}=\sum_{j\in\mathcal{J},j\neq i}F_{ijt}+F_{iot} \quad (9)$$

Finally, we can calculate the outlet mole fraction of B, our controlled variable of interest, from the outlet flowrates of each module that feed into the final outlet. An algebraic mixing of multiple streams is assumed:

$$x^*_{bt}=\frac{\sum_{i\in\mathcal{J}_o}F_{iot}x_{iBt}}{\sum_{i\in\mathcal{J}_o}F_{iot}} \quad (10)$$

Depending on the configuration, only select modules feed into the final outlet, and flowrates between non-connected modules are prohibited:

$$F_{iot} = 0, \quad \forall\, i \notin \mathcal{I}_o \tag{11}$$

$$F_{ijt} \leq F_{ijt}^{max} n_{ijt} \tag{12}$$

The total optimal control problem is to minimize the objective function (1) subject to constraints (2)-(12). As is typical for model predictive control, this formulation can be solved repeatedly in a moving horizon fashion, implementing only the first decided control action, then updating the system's state after a certain amount of time has passed and re-solving the MPC problem. The formulation defines a nonconvex NLP, which can be solved using IPOPT, a well-known fast local NLP solver.

Case Study

The benchmark reactor system studied in this work uses the same parameter values as in the original study (Liu et al. 2009) unless specified below. For the weights of various integral square error and control terms in the objective function, values of $W_x = 10^7, W_T = 1, W_F = 10^7$, and $W_Q = 10^{-5}$ are used. These values help to ensure that all terms are considered roughly equally given the varying orders of magnitude of the different variables. Each reactor module has a volume of 0.17 m^3, such that the total volume of all modules is equivalent to the reactor size tested in the original work (0.5 m^3).

Table 2. Configuration parameters

Configuration	n_{ij}	$\mathcal{I}_o$
Parallel (a)	0 0 0 0 0 0 0 0 0	{1,2,3}
Mixing (b)	0 0 1 0 0 1 0 0 0	{3}
Hybrid (c)	0 0 1 0 0 0 0 0 0	{2,3}
Series (d)	0 1 0 0 0 1 0 0 0	{3}

For the case study analyzed here, we consider a three module system that can operate in any of the configurations specified in Figure 1. Information about the connectivity of the four different modules is given in Table 2. In particular, a parallel configuration (a), a configuration with mixing (b), a hybrid series-parallel configuration (c), and a series configuration (d) are considered. Note that configurations involving splitting are also possible, but neglected in this work due to the extra degree of freedom that would need to be considered (the split fraction).

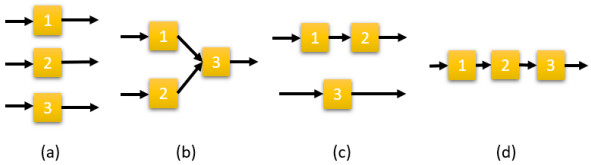

Figure 1. All configurations considered for the 3 module system

For the set point tracking studies performed in this work, we begin with the modular system in parallel configuration (a) at a steady state with outlet mass fraction of B of 0.11 and reactor temperature at 388 K. After 1350 s pass, a set point change in $x_{b,sp}$ occurs. At this time, we consider the cases where the system configuration remains parallel, as well as when it transitions to one of the other three considered configurations. New set points tested range from 0.12 up to 0.26, at a resolution of 0.01. If a configuration change occurs, temperature set point changes also occur in the upstream modules to ensure that the risk of overheating from the series reactors is low. Performance of different configurations is determined by the realized integral square error of x_{bt}^*.

Results and Discussion

In this work, 60 different control simulations are performed, with 4 configuration changes tested for each of the 15 set point changes considered. All optimal MPC problems are solved using Ipopt v0.6.5 in the JuMP v0.22.1 package (Bezanson et al., 2017) in Julia v1.8.1. Computations were performed on a 5.2GHz Intel Core i9-10900 processor.

When analyzing the results of the control simulations, the first thing that is apparent is the extremely poor control performance in large set point changes when transitioning the system to the mixing configuration (b) and the series configuration (d). Representative plots of these poor performances are shown in Figures 2 and 3, respectively. In both figures, it is apparent that the system behaves in an oscillatory manner and that the controller is unable to drive the system to a steady state at its new set point. A look at the process inputs can help to explain why: in both cases the feed flowrates and heating rates in reactor 3, the furthest downstream reactor, saturate at the minimum possible value of zero. Indeed, one can show that to achieve the new composition setpoint, negative heating or flowrates are required for these configurations to reach the desired steady state. This is to ensure that too much C, the undesirable side product, is not formed. Because these two

configurations generally perform very poorly for the set point changes considered, they are not considered in the rest of the analysis.

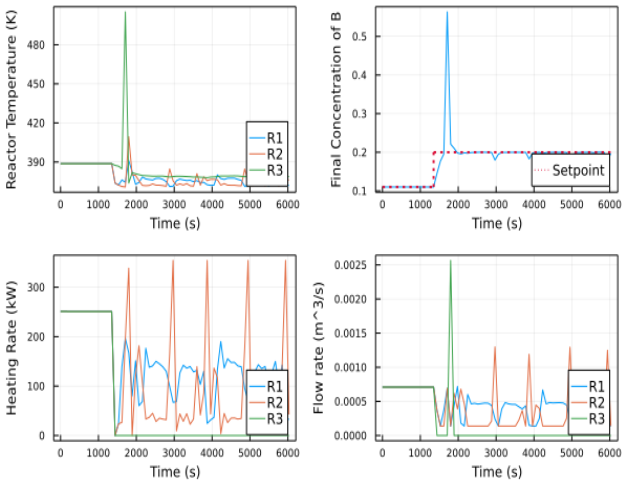

Figure 2. Control performance when the configuration switches from (a) to (b) and the setpoint increases to 0.20

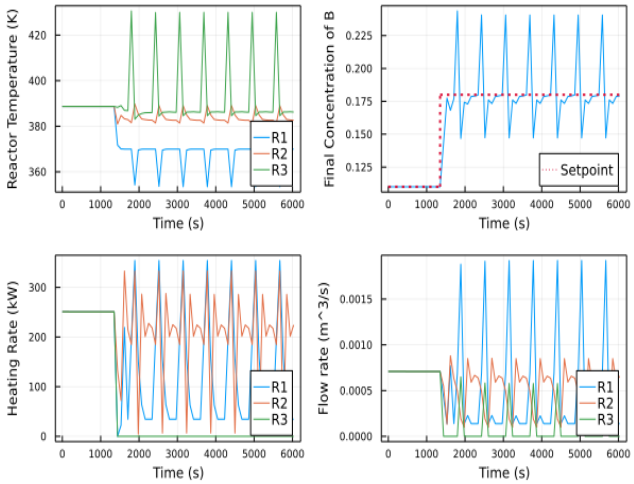

Figure 3. Control performance when the configuration switches from (a) to (d) and the setpoint increases to 0.18

The control performance when keeping the configuration parallel (a) and when converting to the hybrid parallel-series configuration (c), along with the percent improvement from reconfiguration, is shown in Table 3. We note that in general, these two strategies give very similar control performance in all cases, as shown by the representative plots in Figures 4 and 5. In Table 3, we see that keeping the system in the parallel configuration (a) is best for small changes in the set point. Physically, this seems to make sense, as the system is initially at a good steady state in that configuration and the required change to get to the new steady state is not so large. However, as the set point change becomes larger, the hybrid configuration (c) starts to perform relatively better. Indeed, we observe a crossover point at a set point of 0.21 whereby the hybrid configuration (c) becomes the best performer. Physically, the fact that adding a series reactor improves set point tracking for larger concentration set points makes sense, as this can allow for higher conversions due to the increased reactor residence time. Practically, knowledge of the changeover point where the hybrid configuration (b) is very useful, as instead of trying to determine configuration online by solving an MINLP, this offline knowledge can be used to automatically implement a configuration shift for set points above 0.21.

Table 3. Comparison on integral square error for configurations (a) and (c) and % improvement

$\Delta x_{s,m}$	ISE*10^4 (a)	ISE*10^4 (c)	% imp.
0.01	1.03	1.19	-15.6
0.02	4.05	4.61	-13.8
0.03	9.06	10.48	-15.7
0.04	16.60	19.09	-15.0
0.05	28.12	32.35	-15.0
0.06	43.59	47.48	-8.9
0.07	61.65	65.55	-6.3
0.08	81.74	83.75	-2.5
0.09	105.18	105.80	0.6
0.10	136.88	131.91	3.6
0.11	172.50	162.74	5.7
0.12	214.38	198.86	7.2
0.13	260.38	250.73	3.7
0.14	308.96	296.73	4.0
0.15	359.06	346.67	3.5

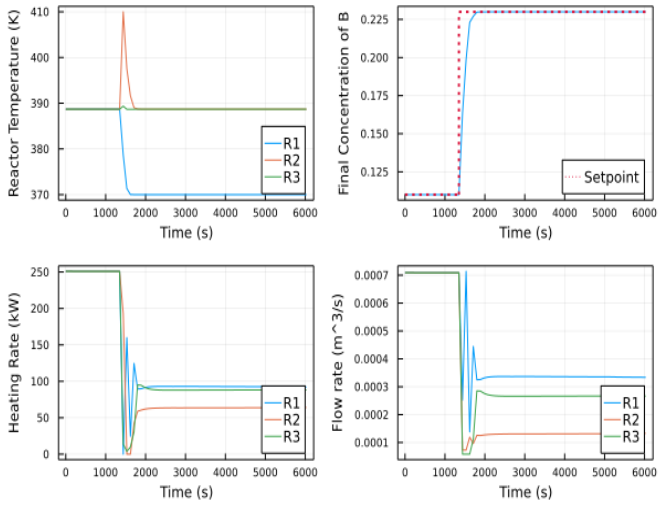

Figure 4. Control performance when the configuration switches from (a) to (c) and setpoint increases to 0.23

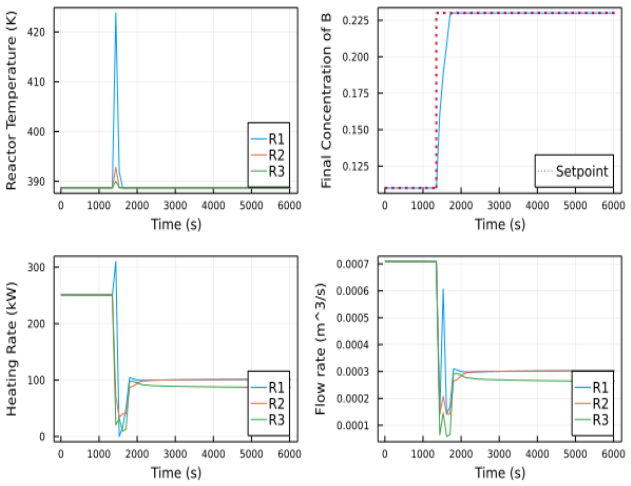

Figure 5. Control performance when the configuration keeps (a) and the setpoint increase to 0.23

As the controller performance for the configurations (a) and (c) looks very similar by analyzing Figures 4 and 5, the set point tracking performance zoomed into where the change occurs is displayed in Figure 6. Here, it is apparent that the hybrid configuration (c) is able to more quickly approach the new set point than configuration (a). However, it is also important to note that the total system throughput, as determined by the sum of fresh feed added to each of the three modules, is larger in the parallel configuration (a). As such, given the similarity in set point tracking performance, it may still be desirable to continue to operate in the parallel configuration (a) even at the highest set points, depending on the process economics.

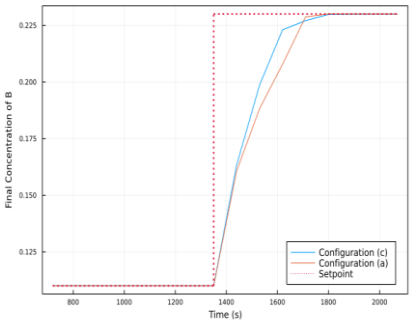

Figure 6. Comparison on the final output concentration between keeping configuration (a) and switching to configuration (c)

Conclusions

In this work, control performance of different configurations of a benchmark modular reactor system was presented. The set point tracking performance of switching configurations was discussed to provide insights that can help prevent needing to solve a challenging MINLP to determine optimal system configurations. In the future, we aim to explore more possible configurations within systems with higher number of modular units, as well as analyzing the disturbance rejection properties of reconfiguration. After fully understanding dynamic characteristics of reconfiguration, we expect to use machine learning tools to develop rules which allow us to perform the selection of system configuration offline, and to keep the complexity of the online optimization problem manageable.

Acknowledgments

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