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Dynamic Simulation and Control of an Integrated Gasifier/Reformer System. Part II: Discrete and Model Predictive Control

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ABSTRACT:

Part I of this series presented an analysis of a multi-loop proportional-integral (PI) control system for an integrated coal gasifier/steam methane reformer system, operating in both counter-current and co-current configurations, for syngas production in a flexible polygeneration plant. In this work, a discrete-PI control system and an offset-free linear model predictive controller (MPC) are presented for the co-current configuration to address process interactions and sampling delay. The MPC model was identified from ‘data’ derived from simulations of the rigorous plant model, with a Luenberger observer augmented to the MPC, to estimate and eliminate plant-model mismatch. MPC offered superior set point tracking relative to discrete-PI control, especially in cases where discrete-PI destabilized the system. The offset-free MPC was developed to solve in less than a second to facilitate online deployment.

Keywords: Steam methane reforming, gasification, dynamic simulation, polygeneration, model predictive control

Nomenclature

Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV</td>
<td>Controlled Variable</td>
</tr>
<tr>
<td>IAE</td>
<td>Integral Absolute Error</td>
</tr>
<tr>
<td>IMC</td>
<td>Internal Model Control</td>
</tr>
<tr>
<td>MPC</td>
<td>Model Predictive Control</td>
</tr>
<tr>
<td>MV</td>
<td>Manipulated Variable</td>
</tr>
<tr>
<td>PI</td>
<td>Proportional-Integral</td>
</tr>
<tr>
<td>RSC</td>
<td>Radiant Syngas Cooler</td>
</tr>
<tr>
<td>S/C</td>
<td>Steam-to-Carbon ratio</td>
</tr>
<tr>
<td>SMR</td>
<td>Steam Methane Reformer</td>
</tr>
<tr>
<td>ZOH</td>
<td>Zero-Order-Hold</td>
</tr>
</tbody>
</table>
### 1 Introduction

In Part I of this series, rigorous dynamic models of a novel integrated coal gasifier/steam methane reformer system (RSC/SMR) were used to develop a control structure and to assess the operability of the system under expected industrial conditions (Seepersad et al., n.d.). The concept for the RSC/SMR was first introduced by Adams and Barton (2011), who illustrated that for a polygeneration plant, improvements in efficiency and profitability can be realized by performing the steam methane reforming (SMR) reactions within the tubes of the gasifier’s radiant syngas cooler (RSC). This configuration capitalizes on available exergy by using the sensible heat of the high-temperature coal-derived syngas to drive the strongly endothermic reaction, producing H₂-rich synthesis gas (syngas) in place of high pressure steam. However, that work only discussed the concept from a systems perspective to determine if it was worth pursuing. The RSC/SMR unit itself was never studied, modeled,
or designed in any degree of detail. Later, a rigorous dynamic model for the system was developed by Ghouse et al. (n.d.-a), and an analysis of the open-loop dynamic behavior of the RSC/SMR is discussed in a follow up paper (Ghouse et al., n.d.-b). In the latter work, the authors identified a number of potential issues that could arise during its operation and that they needed to be considered when constructing a control system.

Next, a proportional-integral (PI) control system was proposed in Part I of this series (Seepersad et al., n.d.) for each of the two design variants of the RSC/SMR: counter-current configuration and co-current configuration. Despite an increasing adoption and interest in advanced control methods, PI control remains the most popular and trusted form of control due to its simplicity, maturity and rapid implementation. As such, PI control was used in Part I to encourage rapid acceptance by industry. Several desirable characteristics for the co-current RSC/SMR system were demonstrated: PI control achieved acceptable responses for set point changes, reliable disturbance rejection, and an ability to maintain tube wall temperatures well below their maximum limits. However, controller interactions were quite significant, and the study utilized continuous controllers, which is a somewhat idealized case and does not take into account hardware limitations of measurement devices.

In more realistic scenarios, the use of digital PI control (instead of continuous PI control) can introduce stability problems into the PI loops. In Part II (this work), the effects of using digital PI control and the impact of differences in sampling times are examined. In addition, a Model Predictive Controller (MPC) is developed which yields better control performance compared to the multi-loop digital PI design. Since the results of Part 1 of this series showed that co-current design is significantly more difficult to control than the counter-current design (slower settling times, more oscillatory behavior), only the co-current design is studied in this work as a “worst case”. As such, the methodology employed herein can be extended to alternative designs. The reader is referred to Part I of this series for a description of the configuration of the RSC/SMR unit, the PI control system configuration, the model and the simulation cases used.

2 Implementation of Digital PI Control

2.1 Digital PI Model and Implementation

The control results presented in Part I of this series can be considered to be the best PI feedback response theoretically achievable due to the continuous signals received by the controllers. In reality, however, the hardware that is utilized to obtain process measurements must invariably take time to process the sample and transmit a measurement signal to the controller. With increasing sampling frequency (decreasing sampling time), the digital PI control performance tends toward continuous PI control. As was used in Part I of this series, the two controlled variables (CVs) defined for this system are: SMR tube exit gas temperature ($T_{gas}$) and SMR tube CH$_4$ slip ($y_{CH_4}$); the manipulated variables (MVs) are: total flow rate into the SMR tube ($F_{SMR}$) and steam-to-carbon ratio ($R_{S/C}$). Considering the CVs defined for this system, the CH$_4$ slip control is more likely to suffer from long sampling times.
The problem is two-fold: firstly, the dynamics of $y_{CH_4}$ ($\tau_p \approx 10$ seconds) are significantly faster than the $T_{gas}$ dynamics ($\tau_p \approx 200$ seconds), where $\tau_p$ represents the time taken for the CV to complete 63.2% of its step-response trajectory; secondly, CH4 slip ($y_{CH_4}$) requires a composition analyzer to measure, which can suffer from long sample times relative to common temperature sensors (Marlin, 2000). As an example, one particular composition analyzer vendor offers a product specifically tailored to industrial NG and syngas applications (Precisive LLC, 2013). The Precisive analyzer feedback frequency can be user-adjusted between one second and five minutes, with longer sample times corresponding to higher measurement accuracy.

The digital PI controller model differs from the continuous PI controller form; the full position version was used in this work (Marlin, 2000):

$$ MV_k = Bias + K_C[E_k + \frac{\Delta t}{\tau_I} S_k] $$

(1)

$$ S_k = \sum_{i=1}^{k} E_i = E_k + S_{k-1} $$

(2)

$$ E_i = SP_i - CV_i $$

(3)

where $K_C$ and $\tau_I$ are the tuning parameters, $E_i$ is the $i^{th}$ sampled error, $k$ is the current sample, $\Delta t$ is sampling time, and $S_k$ represents the summation of past and present errors (analogous to integrating the error in continuous time). As it is not possible to implement a discrete model explicitly within gPROMS (all equations are inherently continuous), the act of sampling and determining the next controller move takes place within a Task (Process Systems Enterprise, 2011). A Task is used in gPROMS to specify an operating procedure, which in this case (see Figure 1 for description) is periodic and constitutes: 1) sampling the CV, 2) implementing a new control action (MV) and 3) maintaining that MV for the controller sample time.

```
WHILE Time < EndTime DO
    SEQUENCE
    REASSIGN
        WITHIN Controller DO
            Error := OLD(SP - CV) ;
            Integral_Error := OLD(Integral_Error) + OLD(Error) ;
            MV := OLD(Bias + Gain * ( Error + (Ts/tau_I)*Integral_Error )) ;
        END
    END
    CONTINUE FOR Controller.Ts
END
END
```

Figure 1: Discrete PI TASK implementation in gPROMS.
This discrete sampling imposes a zero-order-hold (ZOH) on the process measurement. The continuous time signal of the process can be perfectly reconstructed from the discrete measurements, albeit with a phase lag of $\Delta t/2$ from the original signal. As a result, the continuous time tuning parameters must be detuned to account for this phase lag by incorporating the $\Delta t/2$ term into the process dead-time ($\theta_d$). Subsequent simulation tests use the IMC tunings listed in Part 1 of this series (Table 1).

### Table 1: Process and tuning parameters for continuous and discrete PI control with two different sample times (for the co-current configuration).

<table>
<thead>
<tr>
<th></th>
<th>Continuous</th>
<th>$\Delta t = 10 \text{ sec}$</th>
<th>$\Delta t = 30 \text{ sec}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{gas}}$</td>
<td>$K_c$</td>
<td>$\tau_I$</td>
<td>$K_c$</td>
</tr>
<tr>
<td></td>
<td>-94.0</td>
<td>195.0</td>
<td>-91.6</td>
</tr>
<tr>
<td>$y_{\text{CH}_4}$</td>
<td>-23.6</td>
<td>10.2</td>
<td>-17.1</td>
</tr>
</tbody>
</table>

The performance of two different sample time ($\Delta t$) choices was investigated. A sample time of ten seconds was chosen to represent the case where $\Delta t < \tau_{p,y_{\text{CH}_4}}$. A ‘slower’ sample time of thirty seconds was also investigated to represent the case where limitations of the analyzer-feedback result where $\Delta t > \tau_{p,y_{\text{CH}_4}}$. The performance of these two discrete cases relative to continuous PI control is demonstrated next.

### 2.2 Digital PI Results

Several scenarios are selected from those described in Part 1 of this series to illustrate the significance of incorporating sample time on set point tracking and disturbance rejection.

**Case 1a: + 1 percentage point step in $y_{\text{CH}_4}$ set point**

For a step change in the $y_{\text{CH}_4}$ set point, the ten-second PI control performance overall is only slightly different than the continuous case (see Figure 2). The return of $T_{\text{gas}}$ to set point follows roughly the same dynamics as the continuous controller. In the case of $y_{\text{CH}_4}$, a small initial overshoot is quickly corrected to have the CV effectively settled in under two minutes. However, the reduced rate of feedback is detrimental to the thirty-second PI control performance. The composition control in this case is ineffective in meeting the new set point, and destabilizes both controllers in the process. This adverse effect highlights the importance of obtaining sufficiently frequent measurements to ensure system stability under digital multi-loop PI control.
Figure 2: Comparison of continuous and discrete PI (ten and thirty second sampling) control for case 1a (+1 percentage point step in $y_{CH_4}$ set point).

**Case 1b: -10 K step in $T_{gas}$ set point**

For this case (presented in Figure 3), the $T_{gas}$ set point change is represented as a step instead of a ramp in order to obtain a fair comparison across different sampling times. Increasing the sample time causes minor deterioration in temperature control. The effect of discrete sampling is much more evident in the composition control, where using a sample time of thirty seconds results in oscillation in $y_{CH_4}$ that decays at a much slower rate than with the continuous and ten second controllers. The $y_{CH_4}$ CV appears to eventually approach the set point, but this would occur well beyond the simulated 2,000 second window. Such sustained oscillation is unacceptable.
Figure 3: Comparison of continuous and discrete PI (10 and 30 second sampling) control for Case 1b (-10 K step in $T_{gas}$ set point).

Case 4b: 10% reduction in gasifier flow rate ($M_{in}^{i}$)

For this disturbance scenario (Figure 4), all continuous and discrete controllers were able to successfully reject the disturbance effect on $T_{gas}$. Increasing the sample time results in a larger maximum deviation of $T_{gas}$ from its set point, and more pronounced oscillations. For the control of $y_{CH_4}$, as was observed in Case 1b, the amplitude of the deviation increases significantly with increasing sample times, with the thirty-second PI control not being able to settle the CV within the simulated time frame.
As seen in the investigated cases, while the temperature control performance does not degrade significantly by increasing sampling time to thirty seconds, composition control performance exhibits substantial deterioration. With a thirty-second sample time, the PI multi-loop scheme destabilizes the plant for set point changes in composition, even with controller detuning. As such, for the control objectives considered, employing a feedback PI control strategy is inadequate for a sample time of more than ten seconds. These observations promote the need for a more effective method of control to overcome the impact of discrete sampling on the overall stability of the controlled system.

3 Implementation of Offset-Free Model Predictive Control

To obtain improved control performance of the co-current RSC/SMR system in the face of discrete sampling and process interactions, an MPC controller was developed. Having knowledge of the plant dynamics captured within a model predictive framework is expected to yield improved performance relative to PI control. To capture important dynamics in the coal-derived syngas, tube-gas, catalyst, tube wall and refractory wall phases, the number of time-varying states resulting from spatial discretization for the non-linear plant model is in excess of 60,000 variables. Such a model cannot be used as a control model for MPC purposes; a reduction of the model order is necessary. In addition, the vast majority of the states, such as catalyst core temperatures and partial pressures, are not directly measurable. The common practice in this situation is to assume a rigorous non-linear model as the plant (Sanandaji et al., 2011; Wallace et al., 2012), and to develop a data-driven model (typically linear) from plant simulations, with which to implement model-based control techniques.
Within this section, a linear data-driven model is developed in order to implement an MPC controller and interface it with the plant model. While it is desired to characterize the majority of the important non-linear dynamics with the linear model, there will invariably be some degree of offset (plant-model mismatch) due to loss of accuracy. To this end, an offset-free mechanism equipped with a Luenberger observer is used to modify the linear model and eliminate the plant-model mismatch. The principles of this mechanism are discussed in Section 3.1. Following this, the MPC, as implemented, is described in Section 3.3, with an analysis of the MPC results provided in Section 4.

3.1 Offset-Free Mechanism (Observer Design)

In an effort to correct any potential plant-model mismatch, the mechanism described by Wallace et al. (2012) was adopted in this work. To motivate the purpose of implementing an offset-free mechanism, one must first look at what the reduced linear model is trying to represent and achieve. The plant model developed and described in (Ghouse et al., n.d.-a), and simulated in Part 1 of this series, can be characterized by the general non-linear representation:

\[
\dot{x}_{NL} = f(x_{NL}) + g(x_{NL})u \tag{4}
\]

\[
y_{NL} = h(x_{NL}) \tag{5}
\]

where \(x \in \mathbb{R}^n\), \(u \in \mathbb{R}^m\), \(y \in \mathbb{R}^l\) are the vectors of the model states, inputs and measured outputs respectively. In the following analysis and MPC implementation, the measured outputs are \(T_{gas}\) and \(y_{CH_4}\), thus \(y \in \mathbb{R}^2\). For model-based control, it is desired to approximate this system using a linear model, derived from system identification methods, of the general form:

\[
\dot{x}_L = Ax_L + Bu \tag{6}
\]

\[
y_L = Cx_L \tag{7}
\]

where \(A\), \(B\) and \(C\) are coefficient matrices that describe the linearized dynamics of the system. The linear model is developed around the same nominal operating point of the non-linear model; that is to say, the origin of both models should correspond to each other:

\[
\dot{x}_{NL} = 0|_{x_{NL}=0,u=0} \tag{8}
\]

\[
\dot{x}_L = 0|_{x_L=0,u=0}. \tag{9}
\]

At this particular operating point, there is zero offset seen between the linear model and the non-linear plant model, that is to say: \(x_L^0 = x_{NL}^0\). Suppose now, that the same step input \((u_{step})\) is applied to both models. If the linear and non-linear models were allowed to reach a new steady-state, the result derived from (4) and (6) would be:

\[
0 = f(x_{NL}^{ss}) + g(x_{NL}^{ss})u_{step} \tag{10}
\]

\[
0 = Ax_L^{ss} + Bu_{step} \rightarrow x_L^{ss} = -A^{-1}Bu_{step}. \tag{11}
\]

Unlike the steady-state at the origin, the results from the two models will not be the same at the new steady-state (i.e.: \(x_L^{ss} \neq x_{NL}^{ss}\)). This difference is referred to as plant-model mismatch, and arises from the linear model being unable to capture all of the dynamics and interactions of the plant. This plant-
model mismatch may be captured and described as a ‘fictitious state’, designated as \( \theta \), which is estimated using the difference between the outputs of the linear and non-linear models. As the objective is to eliminate plant-model mismatch of the two measured outputs, \( \theta \in \mathbb{R}^2 \). To incorporate \( \theta \) into the identified linear model of equations (6) and (7) yields an augmented model of the form:

\[
\begin{bmatrix}
\dot{x} \\
\dot{\theta}
\end{bmatrix} =
\begin{bmatrix}
A & G\theta \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
x_L \\
\theta
\end{bmatrix} +
\begin{bmatrix}
B
\end{bmatrix} u
\]
\[
y_L =
\begin{bmatrix}
C \\
0
\end{bmatrix}
\begin{bmatrix}
x_L \\
\theta
\end{bmatrix}.
\]

(12)

(13)

Note that in the above expression, \( \theta \) is assumed to not be a function of time, and is not directly influenced by the inputs or states. The discrete implementation of the augmented linear model becomes:

\[
\begin{bmatrix}
x(k+1) \\
\theta(k+1)
\end{bmatrix} =
\begin{bmatrix}
A & G\theta \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
x(k) \\
\theta(k)
\end{bmatrix} +
\begin{bmatrix}
B
\end{bmatrix} u(k)
\]
\[
y(k) =
\begin{bmatrix}
C \\
0
\end{bmatrix}
\begin{bmatrix}
x(k) \\
\theta(k)
\end{bmatrix}.
\]

(14)

(15)

This discrete time augmented model can be compactly represented as:

\[
\tilde{x}(k+1) = \tilde{A}\tilde{x}(k) + \tilde{B}u(k)
\]
\[
y(k) = \tilde{C}\tilde{x}(k),
\]

(16)

(17)

where \( \tilde{A} = \begin{bmatrix} A & G\theta \\ 0 & 1 \end{bmatrix}, \tilde{B} = \begin{bmatrix} B \\ 0 \end{bmatrix}, \tilde{C} = \begin{bmatrix} C \\ 0 \end{bmatrix} \) and \( \tilde{x} = \begin{bmatrix} x \\ \theta \end{bmatrix} \). Ideally, this augmented model represents the non-linear model. An observer is implemented to estimate the states as:

\[
\hat{x}(k+1) = \tilde{A}\hat{x}(k) + \tilde{B}u(k) + L(y_{\text{NL}}(k) - \tilde{C}\tilde{x}(k)),
\]

where the outputs of the observer are subtracted from the plant outputs, and multiplied by \( L \), known as the Luenberger observer gain matrix. The observer error can be denoted as:

\[
e(k+1) = \tilde{x}(k+1) - \hat{x}(k+1).
\]

(18)

(19)

Through substitutions of equations (16) and (18) into (19), the error expression in (19) can be reduced to:

\[
e(k+1) = (\tilde{A} - \tilde{L}\tilde{C})e(k)
\]

(20)

To drive the observer error to zero as \( k \to \infty \), the Luenberger observer poles must be chosen such that the expression \((\tilde{A} - \tilde{L}\tilde{C})\) has all eigenvalues within the unit circle. The observer can be made more aggressive by choosing poles closer to zero. However, due to interfacing the controller and observer with a non-linear model, choosing overly aggressive poles can lead to instability when the model is used in a closed-loop application.
$G_\theta$ and $L$ are the primary tuning parameters associated with the dynamics of the $\theta$ states and their effect on the overall system. Wallace et al. (2012) suggest using the $B$ matrix derived from the linear model as an initial guess for $G_\theta$, treating the $\theta$ states as having the same dynamic effect on the system states as the inputs.

### 3.2 System Identification

The RSC/SMR model represents an infinite-dimensional system, requiring discretization to approximate the system states. The plant model in its full form is too cumbersome to be used for model-based control; to implement MPC, a reduced-order model must be developed. System identification is a black-box, data-driven modeling approach, mapping the inputs ($F_{SMR}$ and $R_{S/C}$) to the outputs ($T_{gas}$ and $y_{CH_4}$). Note that it is not possible to measure the inside of the RSC due to the hazardous conditions, and thus real-time monitoring at any point along the system with the exception of the gas streams at the exit is impossible. Two methods were investigated to obtain a linear model that can approximate the plant response well enough for model-based control, each discussed in turn. Note that the rigorous 2D heterogeneous model with roughly 60,000 variables was used as the “plant response” for all identification steps.

**Method 1: Variable step duration, fixed step size**

The guidelines for this method are described in (Roffel and Betlem, 2004). Each input was moved independently while keeping the others fixed; the input was stepped in alternating directions at increasing pulse widths of $1/4$, $1/3$, $1/2$, $2/3$, $3/4$, $4/4$ and $5/4$ of the time to steady-state (roughly 600 seconds for this system). For the MV $F_{SMR}$, the steps were switched between ± $10$ kmol/hr from its nominal value (21.5 kmol/hr), while $R_{S/C}$ was switched between ± $2$ of its nominal value (3.33 mol H$_2$O/mol CH$_4$). The results of this test are shown in Figure 5.

![Figure 5: System identification test using Method A.](image-url)
Method 2: Fixed step duration, variable step size.

For this method, the step duration was fixed at 1,200 seconds to ensure that all steady-states were captured, irrespective of the step magnitude. The inputs were subjected to a pseudo-random binary sequence (PRBS), multiplied with a random, appropriately scaled number, to generate variable step sizes for the inputs. $F_{SMR}$ was allowed to move within ± 5 kmol/hr from the nominal steady state, while $R_{S/C}$ was allowed to move within ± 2 from steady-state. The results of this identification test are shown in Figure 6.

Using the System Identification Toolbox in MATLAB, a linear state-space model was fit to the data for both identification methods. Using normalized root mean squared error (NRMSE), both methods yielded a fit to the data of about 63 - 77% (where 100% denotes zero error between the predictions and the measurements over the validation dataset). In particular, the sign of the gains for the identified models correctly matched those of the plant; however, the linear models tend to under-predict positive and over-predict negative changes in both outputs. Both methods predict a negative value for $y_{CH_4}$ at instances where the actual CH$_4$ slip approaches zero, which is physically unrealizable, and represents an obvious shortcoming of using a single linear data-driven model to approximate a highly non-linear process. However, this condition never occurred in any of the applications of the linear model described in the following sections.

By augmenting the linear model with the $\theta$ states and Luenberger observer, these deficiencies in the identified model should be negated. The model from methods A and B were compared by equipping them with the offset-eliminating mechanism and observer (tuned using the same observer poles) and

---

Figure 6: System Identification test using Method B.
subjecting to the same input step. The result of implementing a +2 kmol/hr step in $F_{SMR}$ is shown in Figure 7.

![Figure 7: Comparison of identified linear models against non-linear plant output, for a +2 kmol/hr step change in $F_{SMR}$ at $t = 60$ seconds. Both models are equipped with the offset eliminating mechanism. Sample time for both methods is ten seconds.](image)

Both linear models quickly converge to the measured output, effectively matching it after three samples. However, as the end use for this augmented model is MPC (which demands input moves at every sampling instant), it is preferred to implement a model with less severe mismatch at the point of the input step (see inset of Figure 7). The increased severity of the mismatch ‘kick’ in method B’s prediction would have an adverse effect on the stability of the MPC, where each significant input move would produce an initially large offset; the observer would thus have to be detuned, which reduces the speed of the offset-eliminating mechanism. Method A was selected for these reasons, and was found to produce more favourable results in the MPC controller testing stage relative to method B. The model coefficients for the identified model derived through method A are provided in Table 3.1.

### Table 3.1: Linear model coefficients from identification method A.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$[1.020, 97.734; 4.0 \times 10^{-4}, 0.198]$</td>
</tr>
<tr>
<td>B</td>
<td>$[-0.207, 3.404; -0.001, -0.021]$</td>
</tr>
<tr>
<td>C</td>
<td>$[1, 0; 0, 1]$</td>
</tr>
</tbody>
</table>
3.3 Offset-Free Model Predictive Control development

The main criteria influencing the performance of an MPC controller (assuming a satisfactory model) are the objective function used for optimization and the controller tuning parameters. One of the advantages of MPC over conventional PI-control is the ability to tailor this objective function based on the requirements of the end user (a review of MPC formulations can be found in (Qin and Badgwell, 2003)). In this work, the MPC optimization problem was formulated in the standard manner to provide set point tracking and penalize excessive movement of the MVs. The objective function determined by the MPC controller is given by:

$$\min_u \sum_{k=1}^{P} \| \hat{x}(k+1) - x_{sp}(k+1) \|_Q + \sum_{k=1}^{N} \| \Delta u(k) \|_R$$

subject to:

$$u_{\text{min}} \leq u(k) \leq u_{\text{max}}$$

$$\hat{x}(k+1) = \bar{A}\hat{x}(k) + \bar{B}u(k)$$

where $\hat{x}(k)|_{k=1} = [x^0_k \ 0^0_k]^T$

$$\hat{x}(k) = [ \hat{x}_1(k) \ \hat{x}_2(k) \ \hat{\theta}_1(k) \ \hat{\theta}_2(k) ]^T,$$

where $\| \cdot \|_Q$ represents the weighted norm, defined as $\| x \|_Q = x^T Q x$. $Q$ and $R$ are diagonal weighting matrices meant to penalize output and input deviations, respectively.

The guidelines provided by Marlin (Marlin, 2000) provided excellent results and were used for the MPC design of this study, with the tuning procedure by Wallace et al. (2012) used specifically for the tuning of the offset-eliminating mechanism. The following discussion briefly describes the experimentation employed with the various tuning parameters, which led to the choice of acceptable parameters as summarized in Table 3.2.

A challenging aspect of the MPC design for this system is the large difference in process time delay between the two outputs, with $y_{CH_4}$ exhibiting significantly faster dynamics relative to $T_{gas}$. Based on the results of Section 2, the controller sampling time $\Delta t$ was chosen as ten seconds to effectively control this fast output. Choosing $\Delta t > 10$ seconds results in ‘drifting’ of the fast output, which will be difficult to rectify by discrete control action. Also, it will become more difficult for the estimate to converge to the measured output during transients under increased sample times.

Due to the short sampling time, the prediction horizon ($P$) has to be large enough to be able to predict settling of the system; setting $P = 100$ was found to give good MPC performance. The control horizon $N$ is usually chosen to be between one-fourth and one-third of the prediction horizon (Marlin, 2000), but was chosen to be $N = 10$ in this case to balance desired closed-loop performance and optimization computation time (average of 0.375 seconds per optimization solution using $N = 10$). Reducing $N$ produced slightly slower control performance, with the system taking longer to settle after a
disturbance. Increasing N was found to significantly increase optimization computation time, and occasionally produced erratic control movements that intensified plant-model mismatch.

As per the tuning guidelines in (Wallace et al., 2012), the observer tuning matrices $G_θ$ and $L$ were selected based on an assessment of open-loop performance (as discussed in Section 3.2). $G_θ$ was chosen as the B matrix of the identified linear model (Table 3.1) and the observer poles were chosen to be aggressive, yielding the $[L_x L_θ]^T$ matrix as shown in Table 3.2.

Tuning of the $Q$ and $R$ matrices proved especially difficult. In particular, $R$ must be sufficiently large to discourage excessive movement of the inputs but still be scaled relatively to the output weightings. Increasing $R$, which is analogous to reducing controller gains, is necessary in the face of plant-model mismatch and allows the offset-eliminating mechanism to converge to a steady state more swiftly. Improper selection of $R$ relative to $Q$ will result in model estimates ‘chasing’ after the measured outputs, while never truly converging. In initial experimentation to obtain tuning parameters that result in satisfactory MPC performance, the elements of $Q$ were chosen such that the quadratic error term in the objective function for both CVs varied between zero and ten. In addition, $R$ was initially chosen such that the MV penalties in the objective function were large enough to severely restrict movement and deter returning the CVs to set point. Subsequent simulations involved the simultaneous reduction of $R_1$ and $R_2$, whilst adjusting $Q_1$ and $Q_2$, to obtain swift but robust performance in both CVs and effective elimination of plant-model mismatch. The individual elements of $Q$ can be further fine-tuned, based on the relative importance of keeping each CV close to its respective set point.

Through extensive simulation, tuning parameters for MPC design were found to give satisfactory performance, and are summarized in Table 3.2. The MPC with this configuration was tested using several scenarios as explored in Section 4.
### Table 3.2: MPC tuning parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t$ (seconds)</td>
<td>10</td>
</tr>
<tr>
<td>N</td>
<td>10</td>
</tr>
<tr>
<td>P</td>
<td>100</td>
</tr>
<tr>
<td>Q</td>
<td>$\begin{bmatrix} 5 \times 10^{-4} &amp; 0 \ 0 &amp; 10^3 \end{bmatrix}$</td>
</tr>
<tr>
<td>R</td>
<td>$\begin{bmatrix} 4.125 &amp; 0 \ 0 &amp; 0.326 \end{bmatrix}$</td>
</tr>
<tr>
<td>${ u_{\text{min}}, u_{\text{max}} }$</td>
<td>$\begin{bmatrix} 1 \ 2 \end{bmatrix}, \begin{bmatrix} 30 \ 5 \end{bmatrix}$</td>
</tr>
<tr>
<td>$Poles(\begin{bmatrix} T_{gas} &amp; y_{CH_4} &amp; \theta_1 &amp; \theta_2 \end{bmatrix})$</td>
<td>$10^{-5} \times \begin{bmatrix} 4.80 &amp; 0.07 &amp; 4.81 &amp; 0.09 \end{bmatrix}$</td>
</tr>
<tr>
<td>$L_x$</td>
<td>$\begin{bmatrix} 2.02 &amp; -97.73 \ -4.0 \times 10^{-4} &amp; 1.20 \end{bmatrix}$</td>
</tr>
<tr>
<td>$L_\theta$</td>
<td>$\begin{bmatrix} -3.02 &amp; 498.71 \ 0.11 &amp; -30.38 \end{bmatrix}$</td>
</tr>
<tr>
<td>$G_\theta$</td>
<td>$\begin{bmatrix} -0.207 &amp; 3.404 \ -0.001 &amp; -0.021 \end{bmatrix}$</td>
</tr>
</tbody>
</table>
4 Results and Discussion

Case 1a: +1 percentage point step in $y_{CH_4}$ set point

For a change in the $y_{CH_4}$ set point, considerable performance improvement is seen with the MPC controller (Figure 8). Due to the MPC taking both outputs into consideration simultaneously, the flow rate $F_{SMR}$ is aggressively moved at the time of set point change to reduce maximum deviation of $T_{gas}$ from its set point. For $y_{CH_4}$, MPC drives the CV to set point faster than PI control; despite slight initial oscillation around the new set point, $y_{CH_4}$ is effectively settled in approximately 100 seconds. When controlled by the MPC, $T_{gas}$ returns to set point far more quickly than PI control. The aggressive movement of $F_{SMR}$ can be reduced by relaxing the weight of the $T_{gas}$ penalty term in the $Q$ matrix, or by introducing “hard” $\Delta u$ constraints within the MPC formulation.

Case 1b: -10 K step in $T_{gas}$ set point

As with the previous case, the MPC controller takes swifter action than PI control overall due to not having to wait for error to appear between SP and CV. The performance increase is less substantial than in case 1a, with slight oscillations seen in the $T_{gas}$ response. The $F_{SMR}$ MV moves around significantly (see Figure 9), partly due to the speed of response being requested and $\theta$ chasing the plant-model mismatch. Overall MV movement of the MPC case can be reduced by increasing input penalty $R$, but will result in a more sluggish response in the $T_{gas}$ output.
Figure 9: Comparison of PI and MPC (ten second sampling each) control for case 1b (-10 K step in $T_{gas}$ set point).

Case 2a: 50 K increase in gasifier exit temperature ($T_{S}^{in}$)

For this disturbance (Figure 10), the MPC controller performs well with regards to both outputs. As expected, an increase in the gasifier exit temperature causes temperatures in the system to rise, requiring an increase in coolant (SMR) flow. Maximum deviation for $T_{gas}$ using the MPC control is approximately +1.2 K, an 87% reduction from the maximum deviation observed using PI control. Similar reductions were seen with $y_{CH_4}$ control. While the MPC control structure results in less movement in $R_{S/C}$ than PI, the flow rate $F_{SMR}$ experiences increased movement, though not significantly so.
Figure 10: Comparison of PI and MPC (ten second sampling each) control for disturbance case 2a (50 K increase in gasifier exit temperature $T_{\text{S}}^{\text{i}}$).

**Case 4b: 10% reduction in gasifier flow rate ($M_{\text{S}}^{\text{i}}$)**

For this disturbance in the gasifier syngas flow rate, both PI and MPC reduce the SMR flow rate due to the decreased gasifier load, but the MPC MV movement is significantly more oscillatory, especially in $F_{\text{SMR}}$. Maximum CV deviations from set point are drastically reduced from PI control, but experience oscillation that continue past the 2,000 second simulation window. If flow rate disturbances of this magnitude are to be expected, the MPC may need to be detuned (by increasing $R$ or decreasing $Q$) to reduce these oscillations and produce a more desirable response.
Figure 11: Comparison of PI and MPC (ten second sampling each) control for disturbance case 4b (10% reduction in gasifier flow rate $M_3^{in}$).

30 second MPC performance

Suppose that with the sensor and analyzer equipment installed in the plant, the fastest achievable sampling time of the measurements is thirty seconds. Figure 12 and Figure 13 illustrate that, when using thirty second MPC with the same tuning parameters as listed in Table 3.2, stable control performance is still achievable, even in instances where discrete PI control destabilized the system. In particular, by making a step change in the $y_{CH_4}$ set point (Figure 12), there is still rapid approach of the $y_{CH_4}$ CV to set point (case 1a). Recall that for this case (1a), the PI control strategy was completely unstable and therefore unable to achieve the requested set point change for this sample time. The penalty on $T_{gas}$ can be reduced to obtain a less oscillatory but more sluggish return to set point. For thirty second sampled MPC, oscillations in the CVs and MVs are more pronounced for all cases relative to the ten second sampled MPC; this is expected, and detuning of the controller is required as a result.

Figure 12: MPC (thirty second sampling) control for case 1a (+1 percentage point step in $y_{CH_4}$ set point).
Figure 13: MPC (thirty second sampling) control for case 1b (-10 K step in $T_{\text{gas}}$ set point).

The integral absolute error (IAE) metric was used to assess the relative performance of the investigated PI and MPC controllers (Table 3). PI control with a zero second sample time refers to continuous control. For all cases, the thirty second PI control provides the worst performance, especially for $y_{CH_4}$ set point changes. Comparing ten second MPC to ten second PI, the average IAE for $T_{\text{gas}}$ is reduced by 76%, while for $y_{CH_4}$ the average IAE is reduced by 54%. Overall, ten second MPC outperforms continuous PI, with the exception of $y_{CH_4}$ control in the set point change cases. When a sample time of thirty seconds is used, the MPC performance degrades for $y_{CH_4}$ control, but is still within a stable and acceptable range and outperforms thirty second PI in all investigated cases.

Table 3: Comparison of IAE for various PI and MPC sample times.

<table>
<thead>
<tr>
<th></th>
<th>$T_{\text{gas}}$ IAE</th>
<th>$y_{CH_4}$ IAE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Delta t$ (s)</td>
<td>Case 0a</td>
</tr>
<tr>
<td>PI</td>
<td>0</td>
<td>1.58</td>
</tr>
<tr>
<td>PI</td>
<td>10</td>
<td>1.62</td>
</tr>
<tr>
<td>MPC</td>
<td>10</td>
<td>0.19</td>
</tr>
<tr>
<td>PI</td>
<td>30</td>
<td>9.08</td>
</tr>
<tr>
<td>MPC</td>
<td>30</td>
<td>0.39</td>
</tr>
</tbody>
</table>

The MPC control structure allows greater ease and flexibility in adjusting the control structure depending on the objectives. Depending on the end user, it may be desired to have less movement in the MVs while sacrificing set point tracking in the CVs. Through manipulation of the various MPC tuning parameters ($Q, R, L, N, P$) the performance can be tweaked to satisfy user demands based on expected set point changes and plant disturbances. In addition, the MPC structure implemented in this work can be further improved upon by implementing disturbance models to greater counteract gasifier side upsets. However, this requires measurement of the disturbance states, which may not be possible. Additional objectives can also be implemented into the MPC design, perhaps to account for downstream syngas requirements. In particular, the set points of the MPC can be adjusted based on syngas quality requirements, while still providing adequate cooling duty to the coal-derived syngas.
5 Conclusions
For the control of the integrated coal gasifier/steam methane reformer system, the effects of analyzer feedback limitations were addressed, using the co-current base case implementation from Part I of this series. Acceptable discrete feedback PI control performance depends on fast sample times, since the $y_{CH_4}$ dynamic response to system perturbations is twenty times faster than the $T_{gas}$ dynamic response. PI control performance was found to deteriorate substantially with sample times longer than ten seconds. An offset-free, data-driven model predictive controller (MPC) was developed to address this issue, as well as to take process interactions into account. The linear control model was augmented with disturbance states, which were estimated using a Luenberger observer to effectively eliminate plant-model mismatch in the face of unknown disturbances. The MPC controller provided improved set point tracking and settling times versus PI control, especially in the temperature control (76% reduction in IAE relative to PI), which is important for preserving tube life-span. While the MPC easily rejected coal-derived syngas temperature fluctuations, variations in coal-syngas flow rate resulted in oscillatory response, necessitating MPC detuning. MPC control using a sampling time of ten seconds or less provides excellent control of the system; longer sample times (such as thirty seconds) result in drifting of the $y_{CH_4}$ CV, but MPC in this case provides a stable response where multi-loop PI control destabilized the plant. In short, although the linear MPC appears to be more favourable than discrete PI control, there is room for improvement. Because of the high degree of nonlinearity and complexity of the original plant model, a nonlinear MPC strategy may be able to achieve even better performance. This is left for future work.

6 Acknowledgements
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References


PRECISE LLC. (2013). *Precise 5 Hydrocarbon Composition Analyzer*. Woburn, MA: Precise LLC.


