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Online Model Predictive Control of a Nonisothermal and Nonisobaric Membrane Reactor for Water-Gas Shift Reaction Applications

Jacob M. Douglas

Thesis submitted to the
Benjamin M. Statler College of Engineering and Mineral Resources
at West Virginia University

In partial fulfillment of the requirements for the degree of

Master of Science in
Chemical Engineering

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2019

Keywords: Online Model Predictive Control, Quadratic Dynamic Matrix Control, Nonlinear Model Predictive Control, Biomimetic-based Controller cast as MPC

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Abstract

Online Model Predictive Control of a Nonisothermal and Nonisobaric Membrane Reactor for Water-Gas Shift Reaction Applications

Jacob M. Douglas

Modern hydrogen production units are tasked with producing the most hydrogen possible while dealing with flow variations caused by changing power demands. Classical methods for hydrogen production employing the water-gas shift reaction are governed by equilibrium limitations that take effect at high temperatures and high concentrations of H_2 (Georgis, et al., 2014). The implementation of a membrane reactor with temperature control enables the hydrogen concentration and temperature to reach an equilibrium at a higher concentration of H_2 . Another challenge that is prevalent in this process is the cyclical hydrogen demand from changing downstream reforming process conditions. These challenges can be addressed by the implementation of advanced controllers that can cope with dynamic changes associated with different conditions, such as temperature oscillations and mitigation of hot spots.

In this thesis, linear and nonlinear model predictive control (MPC) methods are implemented on a designed water-gas shift membrane reactor model in Aspen Custom Modeler. The implementation aim is to increase the production of hydrogen by considering the temperature control performed by manipulating the flow rates of the coolant entering the cooling jacket at different reactor zones as well as the reactor

sweep flowrate. The control strategies considered for this application are: Quadratic Dynamic Matrix Control (QDMC), Nonlinear MPC (NMPC), and a Biomimetic-based controller cast as MPC (BIO-CS as MPC) (Mirlekar, et al., 2018) . The coolant usage is constrained by the use of quadratic programming (QP), sequential quadratic programming (SQP), or dynamic operations toolbox (DYNOP) solvers, depending on the employed MPC type, to match industrial standards. To mimic industrial conditions, the flowrate of hydrogen in the sweep stream is changed by +15% from its operating steady state. The MPC results that will be discussed show a successful increase in the production of hydrogen with temperature control under changing process conditions.

Dedicated to
My Great Grandmother Helen W. Lee

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Nomenclature

R_{wgs} = Rate law for water – gas shift reaction

k_{eq} = Associated equilibrium constant

v_i = Volumetric flowrate

T_s = Temperature of reactor shell

y_j = Gas component concentration percentage

m_{cat} = Mass of catalyst

v_s = Volume of reactor shell

Q_{diff} = Energy flow due to heat conduction through diffusion

M = Mass flowrate

W_i = Component weight fraction

\tilde{H}_j = Enthalpy

J_i = Molar flux across the membrane

C_i = Component concentration

j_i = Binary parameter that determines the zone of the reactor

Q_m = Species permeance through the membrane

A_s = Area of the Reactor Shell

A_t = Area of the Reactor Tube

$j = \begin{cases} 1, & \text{for the reaction zone} \\ 0, & \text{for the permeation zone} \end{cases}$

U_{mem} = Heat transfer coefficient for membrane

\dot{Q}_{mem} = Energy flow due to heat conduction through the membrane

$Q_{\text{cool},z}$ = Energy flow due to heat conduction through the coolant

U_{cool} = Heat transfer coefficient for coolant

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1. Introduction

Recent market predictions are expecting the world's hydrogen consumption to increase by 17% within the next fifteen years as seen in Figure 1 (Fraile, 2015). The large increase in hydrogen consumption will affect the current largest consumers of hydrogen such as the petroleum and fertilizer industries. In the petroleum industry, the hydrogen is used for hydrocracking crude oil into lighter, higher value hydrocarbons. While in the fertilizer industry, the Haber Process is used to form ammonia.

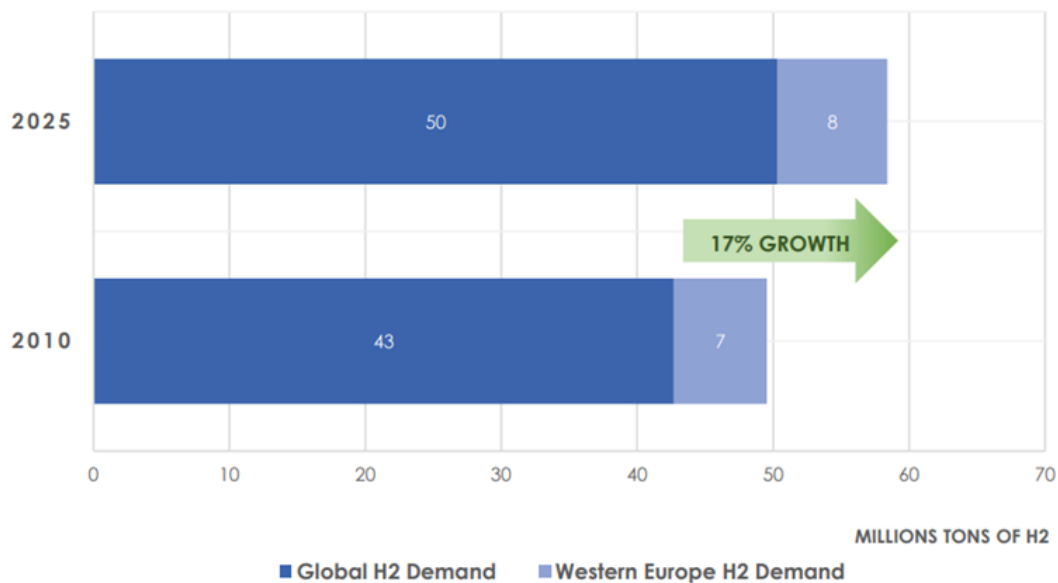


Figure 1. Hydrogen Market Prediction 2010-2025 (Fraile, 2015)

Due to the physical difficulties and high financial expense to transport hydrogen, most companies are forced to produce their required hydrogen on site. The most common industrial method used to produce hydrogen is steam methane reforming. During the steam reforming process, syngas produced from natural gas or petroleum refining is reacted in an exothermic, equilibrium limited reaction known as the water-gas shift reaction as shown in Equation 1 (Zi, 2017).



To keep up with hydrogen demands, the increase of hydrogen production is critical. An innovative solution needs to be introduced that will allow for the equilibrium limitations of the water-gas shift reaction to be overcome toward higher selectivity for hydrogen.

The introduction of membrane reactors could help alleviate this issue by allowing hydrogen to permeate through the membrane. This would enable the equilibrium of the water-gas shift reaction to be shifted toward the production of hydrogen. With this change, it is expected that higher temperatures will occur within the reactor, which could not only damage the membrane, but also reduce the production of hydrogen due to the exothermic nature of the water-gas shift reaction. Additionally, classic Proportional Integral Derivative (PID) controllers used for the traditional industrial process may no longer be able to meet the thermo-regulation requirement for a membrane reactor scheme (Zi, 2017); (Georgis, et al., 2014).

Based on the motivations discussed above, the following objectives are defined for this thesis:

- *Objective #1: Develop a first-principles model for a water-gas shift membrane reactor along with nonlinear and linear system identification models for control purposes.*
- *Objective #2: Create a novel connection between Aspen Custom Modeler / Dynamics and MATLAB through the use of a PI Server.*

- *Objective #3: Implement Linear Model Predictive controllers on an Aspen model to simulate a setpoint change.*
- *Objective 4#: Implement nonlinear model predictive controllers on an Aspen model to simulate a setpoint change.*

The main results of this thesis correspond to: (i) development of a nonisothermal, nonisobaric water-gas shift membrane reactor model in Aspen Plus Dynamics/Custom, (ii) formulation of a strategy to implement custom controllers on Aspen Plus Dynamics/Custom models, (iii) implementation of linear MPC on the water-gas shift membrane reactor Aspen Custom Model, and (iv) implementation of nonlinear MPC on the water-gas shift membrane reactor.

The outline for the remaining sections of this thesis includes a review of literature to expose the gaps in application of model predictive control to a water-gas shift membrane reactor. These gaps are the motivation for implementation of advanced control strategies on a water-gas shift membrane reactor model that will be described in the background. Next, the proposed model equations and linear and nonlinear model predictive control strategies will be discussed. A control framework for online control studies where a plant model will be in Aspen Dynamics/Custom Modeler, while a custom controller will be in MATLAB will then be presented. Finally, results from both linear and nonlinear model predictive control applied online to a water-gas shift membrane reactor will be shown, followed by conclusions and recommendations for the future of the project.

2. Literature Review

In industry, the water-gas shift (WGS) reaction takes place in two packed bed reactors in series as shown in Figure 2. The first reactor operates at a high temperature, thus, shifting the reaction equilibrium towards the production of CO. Subsequently, the second lower temperature reactor shifts the reaction toward the production of H₂. To separate the H₂ from CO and CO₂, a carbon capture unit is utilized (Georgis, et al., 2014)

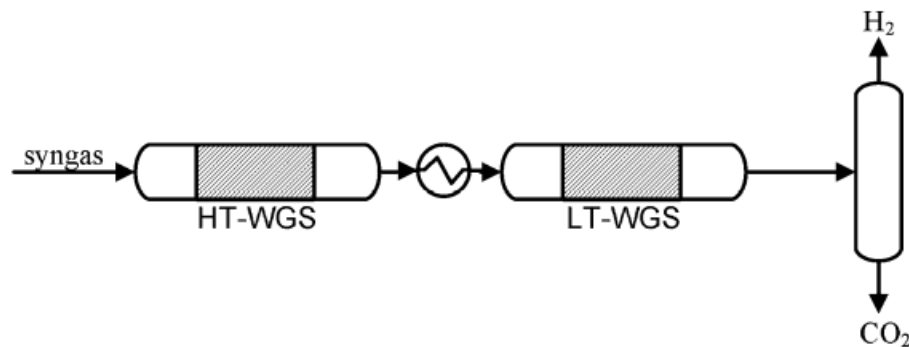


Figure 2. Process Diagram of Traditional Water-Gas Shift Reactor (Georgis, et al., 2014)

When using a typical membrane reactor design, as shown in Figure 3, the area used for permeation outweighs the surface area needed for thermal regulation. A coolant zone maybe placed in the center of the reactor but would not offer substantial thermal regulation for most industrial purposes (Georgis, et al., 2014).

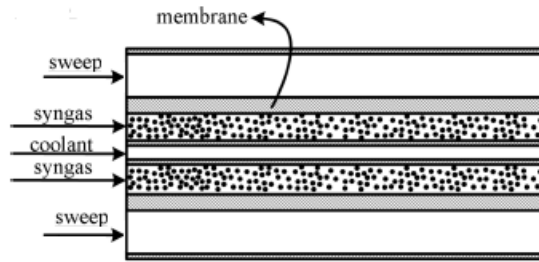


Figure 3. Co-current Membrane Reactor from Literature (Georgis, et al., 2014)

To address the thermal regulation issue, a design was proposed, shown in Figure 4, where the reactive section was moved to the outer shell while the sweep would be placed on the inner section. This would allow a cooling jacket to be attached to the exterior of the reactor (Georgis, et al., 2014).

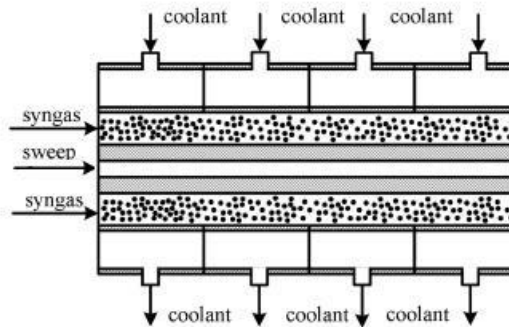


Figure 4. Membrane Reactor with Thermal Regulation Design (Georgis, et al., 2014)

In literature, several different control strategies have been implemented on this water-gas shift membrane reactor such as PID and a nonlinear controller (Zi, 2017); (Georgis, et al., 2014). These control strategies have resulted in sluggish control responses to this demanding control problem. To solve this, first and higher generation model predictive control strategies have been discussed as future works in these references, but they have never been either attempted or documented.

The model predictive controllers that will be discussed in this thesis are: quadratic dynamic matrix control (QDMC), nonlinear model predictive control (NMPC), and Biologically-Inspired Optimal Control Strategy (BIO-CS).

QDMC is a second generation MPC that was designed in the 1980's. This control strategy utilizes a linear step response model being used to represent the plant and a predictive horizon used to predict future outputs, as demonstrated in Figure 5 (Qin & Badgwell, 2003). The QDMC is a constrained control strategy, which produces an optimization problem where optimal inputs are calculated as the solution of a quadratic program (QP) minimization (Bequette, 1998).

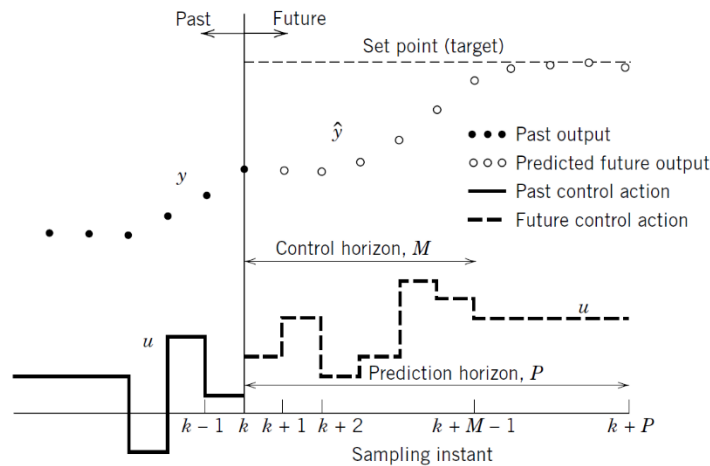


Figure 5. Formulation with Prediction and Control Horizon for QDMC (Bequette, 1998)

NMPC is a fourth generation MPC theorized in the late 1990's that uses advanced optimizers, such as sequential quadratic programming (SQP) to impose both linear and nonlinear constraints on states of inputs of a system. NMPC may also

involve the use of a nonlinear model, in which output predictions more accurately represent plant behavior (Bequette, 1998).

BIO-CS when cast as MPC is part of the newest generation MPC developed by Dr. Mirlekar and the CODES research group at West Virginia University in the late 2010's. BIO-CS uses the Dynamic Optimization toolbox (DYNOPT) as well as multiple agents to calculate the optimal control trajectory for a given process as well as impose both linear and nonlinear constraints (Mirlekar, et al., 2018).

3. Background

3.1 WGS Membrane Reactor Model

The main contributions for the WGS membrane reactor modeling have been detailed in (Georgis, et al., 2014). Those contributions have been summarized below and have been essential to the development of this research.

WGS is the final step of the steam methane reforming process where CO and H₂O are reacted in a reversible reaction to form CO₂ and H₂ as seen in Equation 1. The reversible reaction rate law can be seen in Equation 2.

$$R_{wgs} = -v_i k_{eq}(T_s) \left(P_s^{(0.5 - P_s/500)} \right) \left(y_{s,CO} y_{s,H_2O} - \frac{y_{s,CO_2} y_{s,H_2}}{K_{eq}(T_s)} \right) \left(\frac{m_{cat}}{V_s} \right) \quad (2)$$

An one-dimensional dynamic model was developed by (Georgis, et al., 2014) with the following assumptions: ideal gas behavior and negligible axial diffusion. The mass conservation for the system is shown in Equations 3-5 where the simultaneous mass transport and reaction is described by Equation 3 and the permeation through the membrane is given by Equations 4 and 5. The boundary conditions used to solve Equation 3 can be seen in Equations 6-9.

$$\frac{\partial C_{jn+i}}{\partial t} = -1^{(j+1)} \left(-\frac{\partial F_{jn+i}}{\partial V_j} + J_i + j R_{wgs} \right) \quad (3)$$

$$J_i = \begin{cases} \frac{d_t \pi}{A_s} Q_m (P_{i,s} - P_{i,t}) & \text{for } j = 1 \end{cases} \quad (4)$$

$$J_i = \begin{cases} \frac{d_t \pi}{A_t} Q_m (P_{i,s} - P_{i,t}) & \text{for } j = 0 \end{cases} \quad j = \begin{cases} 1, & \text{for the reaction zone} \\ 0, & \text{for the permeation zone} \end{cases} \quad (5)$$

$$C_{t,i} (0, t) = C_{s,i}^{in} \quad (6) \quad C_{s,i} (z, 0) = C_{s,i}^0 \quad (7)$$

$$C_{t,i} (0, t) = C_{t,i}^{in} \quad (8) \quad C_{t,i} (z, 0) = C_{t,i}^0 \quad (9)$$

The energy conversation equation is described by the partial differential equation seen in Equation 10. The boundary conditions used for Equation 10 can be seen in Equations 11-14. Equation 15 is responsible for modeling the energy generated by the reaction, energy being transported through the membrane, and the energy being extracted due to the cooling jacket (Georgis, et al., 2014). The energy balances for the cooling jacket sections is considered in Equation 16, with the initial conditions in Equation 17.

$$\frac{\partial H_j}{\partial t} = -1^{(j+1)} \left(-\frac{\partial F_j MW_j \tilde{H}_j}{\partial V_j} - \frac{Q_{diff}}{A_j} - \frac{Q_{mem}}{V_j} - j \frac{Q_{cool,z}}{V_j} \right) \quad (10)$$

$$T_s (0, t) = T_s^{in} \quad (11) \quad T_s (z, 0) = T_s^0 \quad (12)$$

$$T_t (0, t) = T_t^{in} \quad (13) \quad T_t (z, 0) = T_t^0 \quad (14)$$

$$\tilde{H}_j = \sum_{i=1}^n w_i \left(\Delta H_{f,i}^{\circ} + \int_{T_{ref}}^T c_{p,i}(\tilde{T}) d\tilde{T} \right) \quad (15)$$

$$\frac{dH_{cool,z}}{dt} = (F_{cool,z}^{in} MW_{cool,z}^{in} \tilde{H}_{cool,z}^{in} - F_{cool,z} MW_{cool,z} \tilde{H}_{cool,z}) + \dot{Q}_{cool,z} \quad (16)$$

$$T_{cool,z} (0) = T_{cool,z}^0 \quad (17)$$

$$\dot{Q}_{cool,z} = U_{cool} \pi d_s \int_{l_{i,z}}^{l_{f,z}} (T_s(z) - T_{cool}) dz \quad (18)$$

$$Q_{diff} = \sum (J_i MW_i) \tilde{H}_j \quad (19)$$

$$Q_{mem} = U_{mem} A_t (T_s(z) - T_t(z)) \quad (20)$$

For the considered membrane reactor with a length of 30 cm, the WGS reaction takes place in the first 5-10 cm of the reactor, which causes a severe temperature spike at the beginning part of the reactor. This temperature spike can cause membrane damage if it can exceed 700°C (Zi, 2017). Classic PID and nonlinear controllers have been attempted to try and mitigate this temperature spike, at the expense of having sluggish responses in setpoint changing scenarios. To solve this challenging control problem more advanced controllers are needed.

3.2 Advanced Control Strategies

The control strategies considered for implementation in this work are the quadratic dynamic matrix control (QDMC), nonlinear model predictive control (NMPC), and Biomimetic-based controller cast as MPC (BIO-CS as MPC) (Mirlekar, et al., 2018). Each of these controllers will be responsible for calculating new inputs to move the process from its initial condition to a different desired condition.

QDMC is a second-generation linear model predictive control strategy that uses a model obtained from step response (Qin & Badgwell, 2003). QDMC utilizes quadratic programming (QP) to calculate the inlet changes needed to reach the desired steady-state target. With the use of QP, linear constraints can be applied to the process. The equation used for the QP along with the linear constraints can be seen in Equation 21 (Bequette, 1998).

$$\hat{y}^c(k+j) = \sum_{i=1}^j S_i \Delta u(k-i+j) + \sum_{i=j+1}^{N-1} S_i \Delta u(k-i+j) + S_N u(k-N+j) + \hat{d}(k+j) \quad (21)$$

$$\min \Phi = \frac{1}{2} \Delta u_f^T H \Delta u_f + c^T \Delta u_f$$

NMPC is a nonlinear model predictive control strategy that requires either a nonlinear solver such as sequential quadratic programming (SQP) with nonlinear constraints or a nonlinear model. The SQP objective function and the disturbance mitigation terms used in this control strategy can be seen in Equation 22 (Bequette, 1998).

$$\hat{y}^c(k+j) = \sum_{i=1}^j S_i \Delta u(k-i+j) + \sum_{i=j+1}^{N-1} S_i \Delta u(k-i+j) + S_N u(k-N+j) + \hat{d}(k+j) \quad (22)$$

BIO-CS can be a linear or nonlinear model predictive control strategy, depending on the types of models and constraints, that requires a system of ordinary differential equations model. This control strategy utilizes the DYNOPT solver to calculate the optimal control strategy. The objective function used in the BIO-CS can be seen in Equation 23 (Mirlekar, et al., 2018).

$$\min_{\mathbf{u}(t)} J = \int_{t_i}^{t_f} \|\mathbf{y}(t) - \mathbf{y}_{sp}\|^2 + \|\mathbf{u}(t) - \mathbf{u}^-(t)\|^2 dt \quad (23)$$

4. Proposed Approach

One of the main objectives in this research is to develop a model in Aspen for a WGS membrane reactor to compare different linear and nonlinear MPCs. This study will lead to the discovery of which MPC strategies are possible for online use in the developed model.

4.1 WGS Membrane Reactor Modeling

The water-gas shift membrane reactor design selected for this application is shown in the schematic in Figure 6. The design for this study was inspired by a model documented in literature (Georgis, et al., 2014) and was recreated in Aspen Custom Modeler V9. The design selected allows higher conversions to be reached due to the ability for greater thermal regulation compared to other literature models. The dimensions for this reactor are as follows: diameter of the cooling jacket of 4.00cm, diameter of the reactive shell of 2.88 cm, the diameter of the inner sweep tube of 2.28 cm, the length of the reactor of 30.0 cm, and each cooling zone is 5 cm in length.

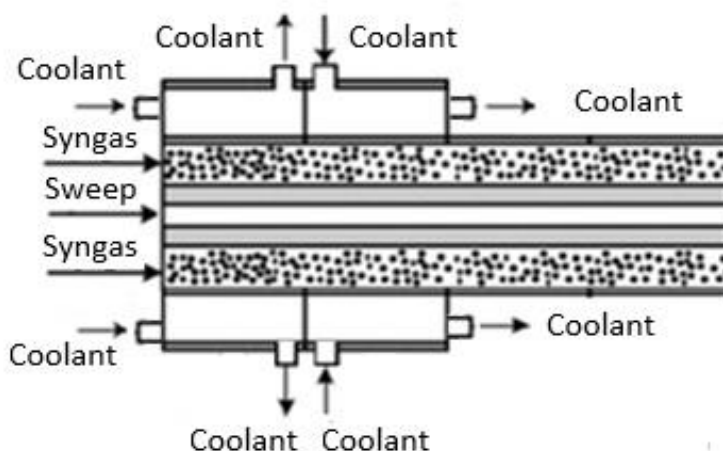


Figure 6. Water-Gas Shift Membrane Reactor Schematic

The nonisothermal, nonisobaric, dynamic water-gas shift membrane reactor model is developed in Aspen Custom Modeler V9 using the mass and energy balance equations for this model that are shown in Equations 2-20.

For the control studies to be completed, first the decision of the control structure will need to be made. When deciding the manipulated variables, one has to take into consideration what variables one will be able to manipulate in industry. In this case, the inlet flowrate of the syngas should not be selected as a manipulated variable as in industry this membrane reactor unit will have to be able to deal with the amount of syngas required from the upstream steam methane reforming unit. The manipulated and controlled variables selected for this study can be seen in Table 1.

Controlled Variable	Manipulated Variable
Reactive Zone #1 Outlet Temperature (y_1)	First Cooling Jacket Coolant Molar Flowrate (u_1)
Reactive Zone #2 Outlet Temperature (y_2)	Second Cooling Jacket Coolant Molar Flowrate (u_2)
Concentration of H_2 in the Sweep Section (y_3)	Total Molar Flowrate of Steam Entering the Sweep Section (u_3)

Table 1. Controlled and Manipulated Variables for the WGS Membrane Reactor

To implement MPC strategies on the Aspen Custom Model, a reduced model for control purposes will need be created by the use of system identification. To test the effects of the variables on the online model, an input and output feasibility mapping will need to be completed. For control purposes, the two models that will be used are a linear model using ARX (MATHWORKS, 2019) and a nonlinear model using NARX (MATHWORKS, 2019). The input-output mapping needs to be completed

using the original and the two reduced models and a common output point among all the models must be picked to ensure setpoint achievability with minimal offset between the predicted model and the online Aspen Model.

The nonlinear version of the model is created by applying step response excitations to the system. The data collected from the step tests are applied to NARX equations found within the MATLAB System Identification Toolbox (MATHWORKS, 2019).

The linear version of the model is created by taking a smaller step test with a range of data points that includes the initial starting position of the simulation and the region of the desired output. The data collected from the step tests are applied to ARX equations found within the MATLAB System Identification Toolbox. The ARX equations are then transformed into a state space matrix (MATHWORKS, 2019).

4.2 Connection Between Aspen Plus Custom Modeler / Dynamics and MATLAB

To apply custom controllers to first-principles models in Aspen, a control software framework is created as shown in Figure 7. To create this framework, data would need to be able to flow bidirectionally. To solve this issue, the Aspen Custom model is opened in the Aspen Operator Training Simulator (OTS) to allow the Aspen Custom Model data to be sent to an OPC DA 3.0 server. From here, a read/write OPC DA interface provided by OSIsoft is used to send data from the OPC DA server to a PI Server where the data is securely recorded. The data from the PI Server is sent to MATLAB using Web API. Control actions are then calculated in MATLAB and sent

back to the PI Server through Web API. The PI Server updates the OPC DA server, which in turn updates the Aspen Custom Model. The interface between Aspen, OSIsoft PI server, and MATLAB can be seen in Figure 8.

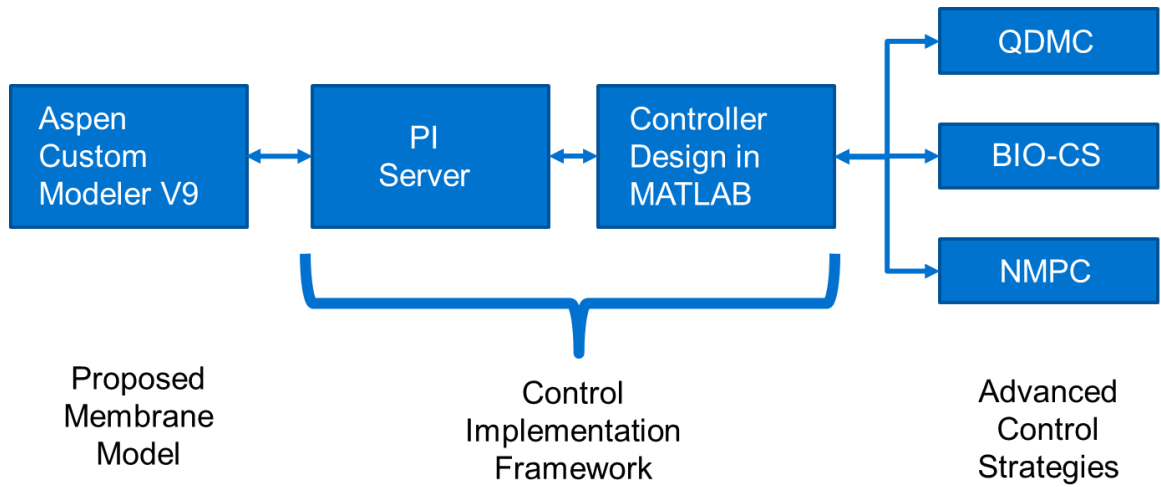


Figure 7. Software Framework for Control Implementation

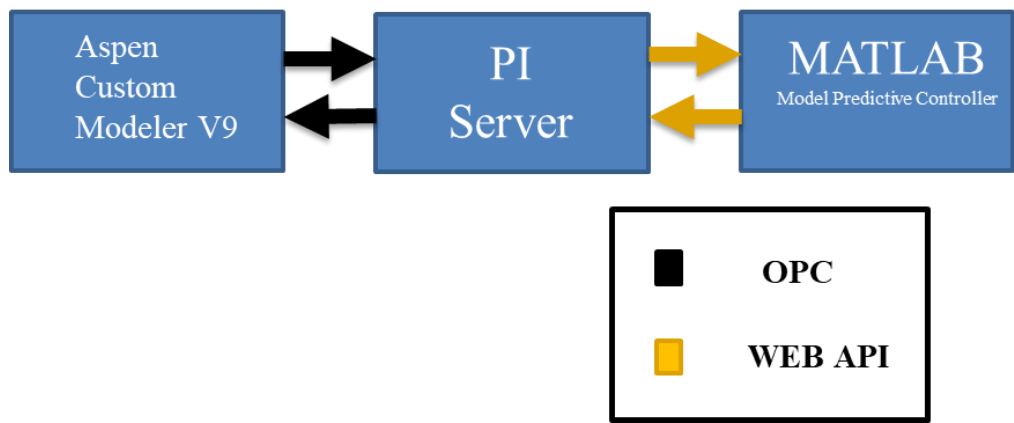


Figure 8. Aspen – PI Server – MATLAB Interface

4.3 Assessment of Linear Model Predictive Controllers on Aspen Model to Simulate Setpoint Change

To determine which linear MPC controllers would be viable, different controllers needed to be tested on the Aspen Model. For this research, the linear MPC controllers QDMC and BIO-CS cast as MPC are considered. The controllers are tested to see how large of a plant-model mismatch occurred, how fast the controller can achieve steady state conditions, and how much computational time the new controllers need for calculations. Feasibility is determined if the controller is able to get to steady state and if the average controller computational time per move is less than or equal to 1 sample/unit time. These controllers are expected to have a fast-computational time as they are based on a linear model.

4.4 Assessment of Nonlinear Model Predictive Controllers on Aspen Model to Simulate Setpoint Change

For this research, the nonlinear MPC controller that was chosen is NMPC. The controller would be tested to see how large of a plant-model mismatch occurred, how fast the controller is able to achieve the new steady state, and how much computational time the controller needed. Feasibility is determined if the controller is able to get to steady state and if the average controller computational time per move is less than or equal to 1 sample/unit time. The nonlinear MPC strategies are expected to have a higher computational expense but are expected to reach the desired steady state faster due to the utilization of more advanced optimizers used in calculating the optimal inputs.

5. Results and Discussion

5.1 WGS Membrane Reactor Model

Several different models are needed to be used for control and model predictions within both the linear and nonlinear model predictive control strategies. A linear, state-space model is needed for the QDMC and the BIO-CS, while the NMPC required a nonlinear identified model. For BIO-CS, the linear state-space model is transformed into a system of differential equations. To accurately represent the application of these control strategies to a plant, the first-principles PDE model in Aspen Custom Modeler is employed for the plant representation.

5.1.1 Aspen Custom Model

A first-principles model for the water-gas shift membrane reactor is created in Aspen Custom Modeler V9. This model is then checked for both concentration and temperature profiles by a comparison of the models with literature.

5.1.1.1 Concentration Profile from Aspen Model

Using the water-gas shift reactor model from literature that was recreated in Aspen Custom Modeler V9. An open loop case shows a very rapid increase in the hydrogen concentration in the sweep gas that can be attributed to the rapid production of hydrogen within the first 5 cm of the reactor. The concentration profile of both the reaction and sweep sections can be seen in Figure 9.

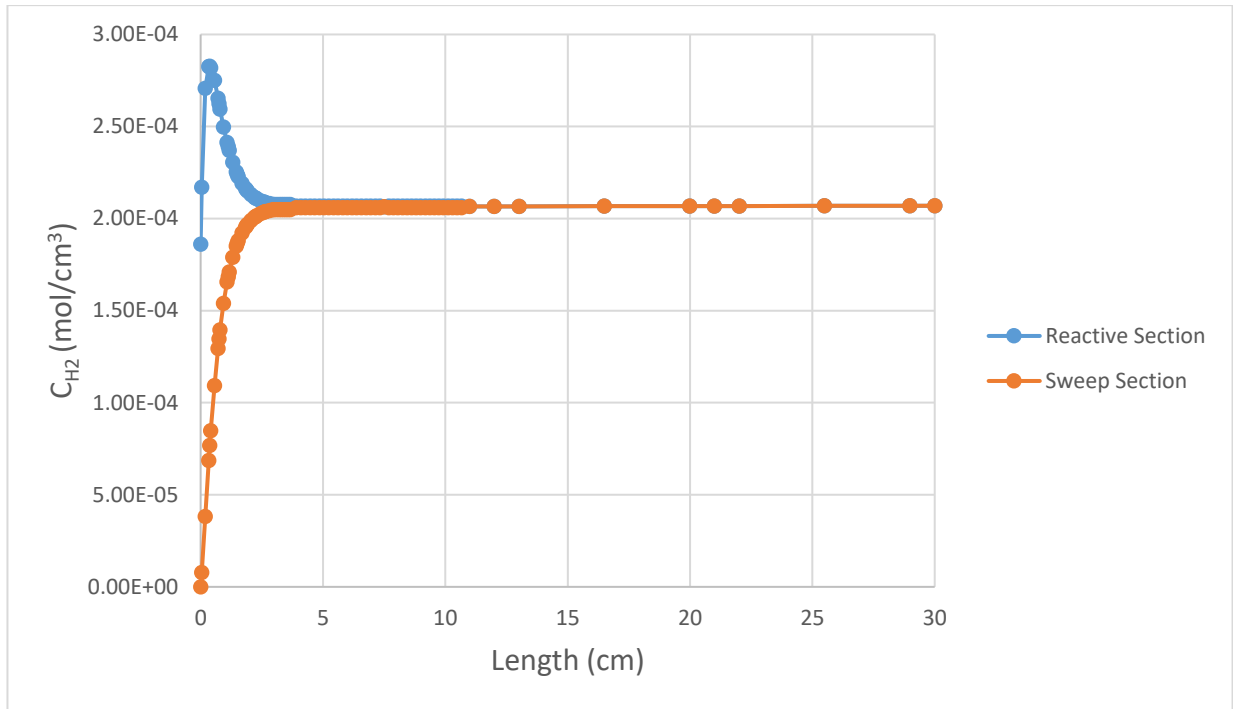


Figure 9. WGS Membrane Reactor Open Loop Concentration Profiles from Aspen Model

5.1.1.2 Temperature Profile from Aspen Model

The temperature profile for the Aspen Custom WGS membrane reactor's open loop case seen in Figure 10 shows a drastic temperature spike within the first 5cm of the reactor. This drastic temperature rise is caused by the high reaction rate that takes place in this section of the reactor. With the temperature of the reactor nowhere near the maximum allowable temperature of 700°C, a setpoint where a higher reaction rate takes place is possible.

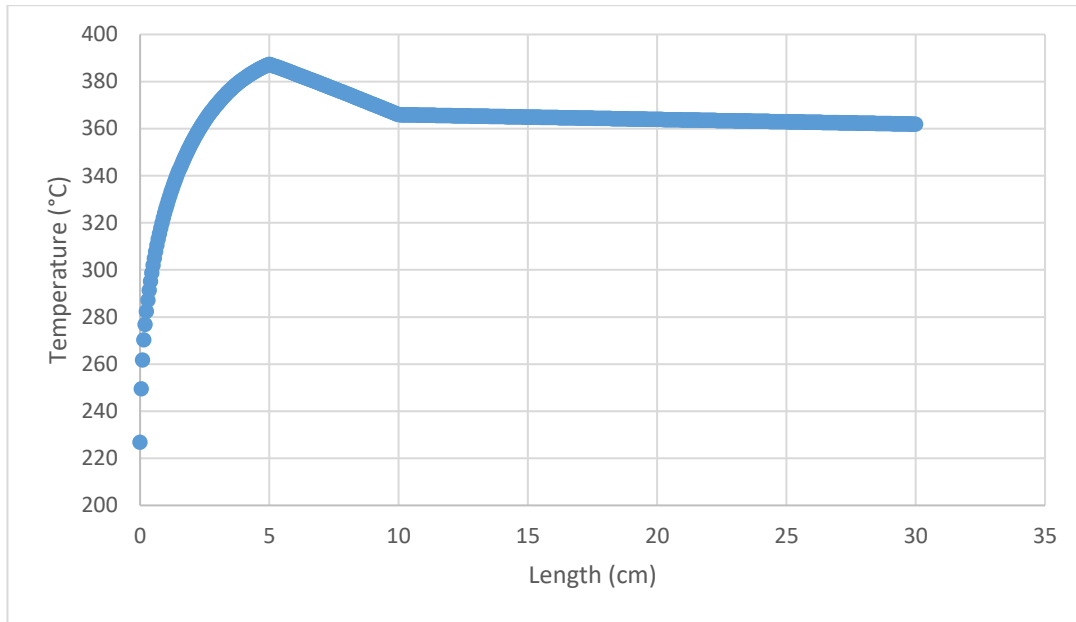


Figure 10. WGS Membrane Reactor Open Loop Temperature Profiles from Aspen Model

5.1.2 Linear Identification Model

All linear model predictive control strategies require a linearized system identification model for control purposes. The creation of this linear model is completed by implementing a step test on the WGS membrane reactor PDE model from Aspen Custom Modeler. For this step test, the molar flowrate for the coolant entering reactive section 1 (u_1) is stepped up by .02 kmol/hr from its initial point of .1 kmol/hr. The coolant molar flow rate in zone 2 (u_2) is also stepped up by the same amount and finally the sweep molar flowrate (u_3) is increased by 15%.

The input and output data gathered from the step tests are then applied to the continuous polynomial ARX model inside the MATLAB System Identification Toolbox. This produced polynomial functions that represent the system.

The polynomial equations acquired from the ARX model are then transformed into a state-space format using the idss function in MATLAB. The state-space model acquired can be seen in Equations 24-27. This linear model is able to accurately represent the plant model with high correspondence to the state-space model by comparing to the data gathered from the Aspen Model step tests. The ARX percent fit per output can be seen in Table 2.

Table 2. ARX output best fit comparison to Aspen Model

ARX vs Aspen Model	
	Percent Fit
Reactive Zone #1 Outlet Temperature (y1)	90.41
Reactive Zone #2 Outlet Temperature (y2)	89.66
Concentration of H2 in the Sweep Section (y3)	91.22

$$A = \begin{bmatrix} 0.99991 & 0.00635 & -0.00782 \\ 0.09895 & 0.88019 & 0.03002 \\ 0.07546 & 0.02759 & 0.89646 \end{bmatrix} \quad (24)$$

$$B = \begin{bmatrix} -0.00081 & -0.00003 & -0.00024 \\ 0.00908 & -0.00456 & 0.00121 \\ -0.00128 & -7.527E-06 & 0.00103 \end{bmatrix} \quad (25)$$

$$C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (26) \quad D = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (27)$$

This linearized model is then tested with the same inputs as the Aspen Custom Model to determine the achievable regions for both models. The comparison result of this mapping is presented in Section 5.1.4.

5.1.3 Nonlinear Identification Model

For a model predictive controller to be nonlinear, either the model used needs to be nonlinear, the optimizer needs to be nonlinear, or the constraints applied to the optimizer need to be nonlinear. In the case of the NMPC used in this research, it was decided to use a nonlinear model to attempt to minimize the potential plant-model mismatches.

The input and output data gathered from the step test is applied to the NARX model inside of the MATLAB System Identification Application. This model is found to be extremely accurate with high correspondence to the output space considering the validation of the state-space model against the data gathered from the Aspen Model step tests. The NARX percent fit per output can be seen in Table 3.

Table 3. NARX output best fit comparison to Aspen Model

NARX vs Aspen Model	
	Percent Fit
Reactive Zone #1 Outlet Temperature (y1)	98.36
Reactive Zone #2 Outlet Temperature (y2)	94.99
Concentration of H2 in the Sweep Section (y3)	94.67

5.1.4 Comparison between Linear, Nonlinear, and PDE model

In Figures 11 and 12, an input-output mapping result for the Aspen Custom, NARX, and ARX models are shown. The outputs in Figure 12 show little discrepancy between the Aspen Model and the NARX model, but the ARX model can vary significantly as we move farther away from the initial point. From this result, a region

in which a common output between the models occurs was chosen and is represented by the red circle in Figure 12.

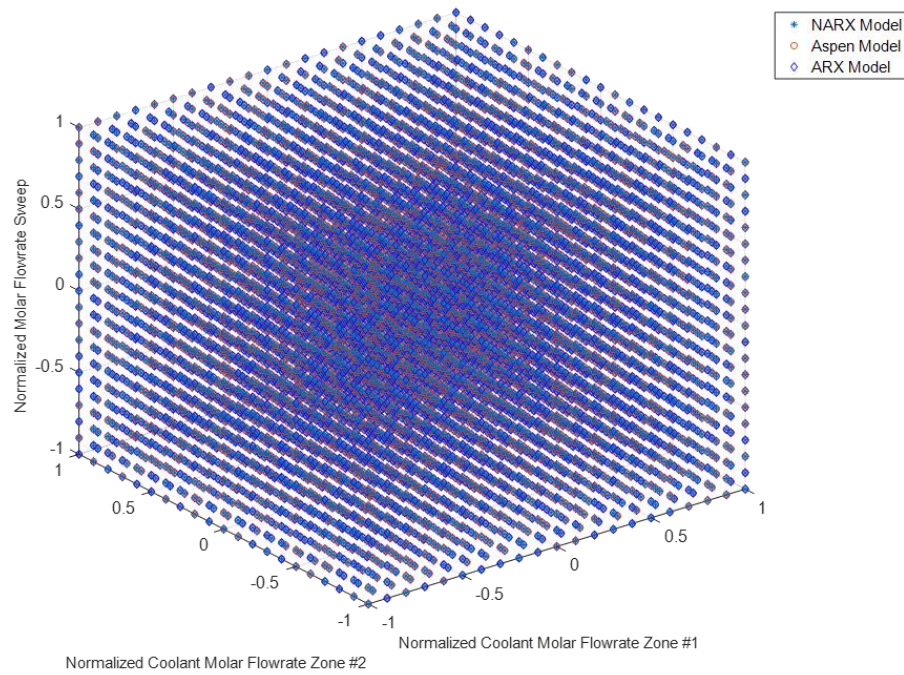


Figure 11. Input for Aspen Custom, ARX and NARX Models

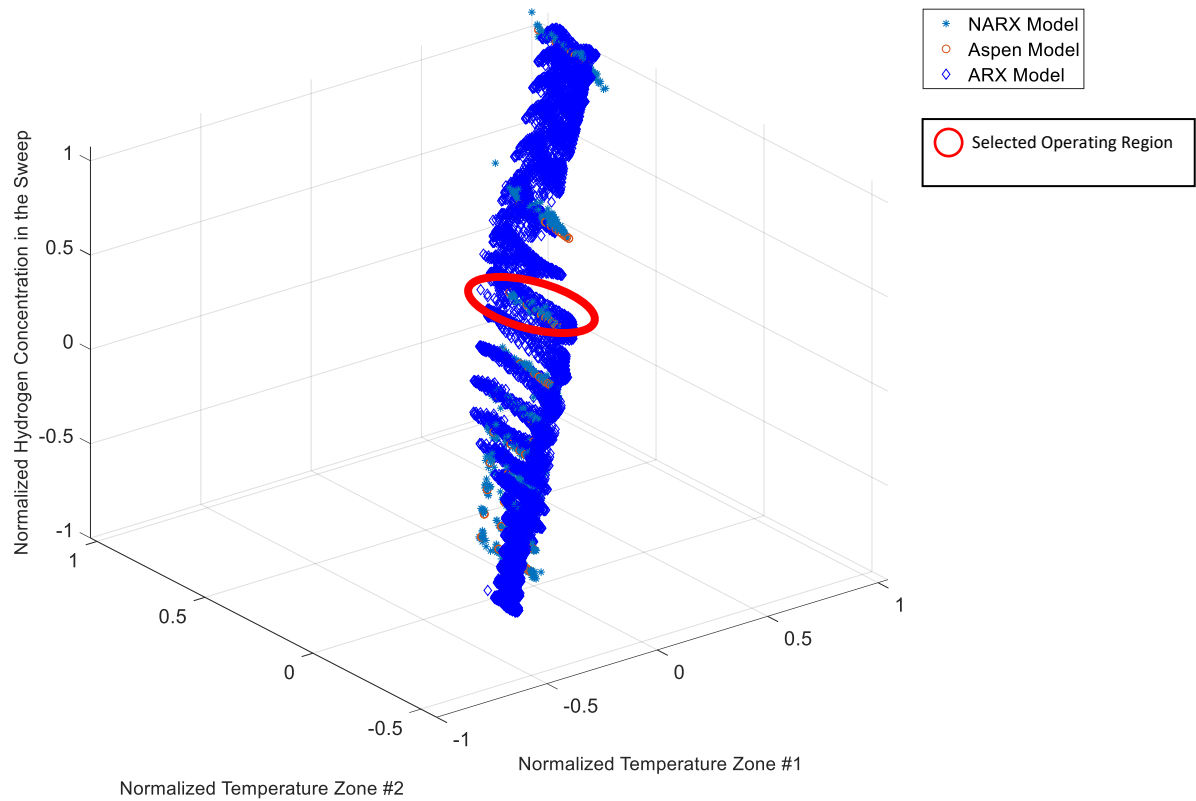


Figure 12. Aspen Custom Model Output vs ARX and NARX model Output

5.2 Connection between Aspen Plus Custom / Dynamics and MATLAB

A connection between the water-gas shift membrane reactor in Aspen and the MPC controllers in MATLAB was created. Data from the Aspen Model was able to be successfully sent and received over the OPC DA server to an OSIsoft PI Server, to the MATLAB control strategy.

5.3 Implementation of Linear Model Predictive Controllers on Aspen Model to Simulate Setpoint Change

The goal for the model predictive control strategies is to increase the outlet hydrogen concentration in the sweep stream by 15% while also making sure the temperatures of outlet first reactive zone is of 585.24°C and the temperature of the outlet second reactive zone is of 507.52°C. These setpoints selected for temperature are based on the setpoint achievability mapping discussed in Section 5.1.4. For each control strategy, an input constraint range of 0 to 0.060 kmol/hr was applied to inlet of coolant into the cooling jackets, as well as the sweep gas was constrained within the range of 0 to 0.178 kmol/hr.

5.3.1 QDMC

The first model predictive control strategy attempted on the WGS membrane reactor was QDMC. For this strategy, a control action was taken every 1 second. The closed-loop result for QDMC can be seen in Figures 13 and 14. The controller was able to get to the desired setpoint, but the controller took around 60 seconds to reach steady state. This controller was applied to the Aspen Custom Model using the software connection described in Section 5.2.

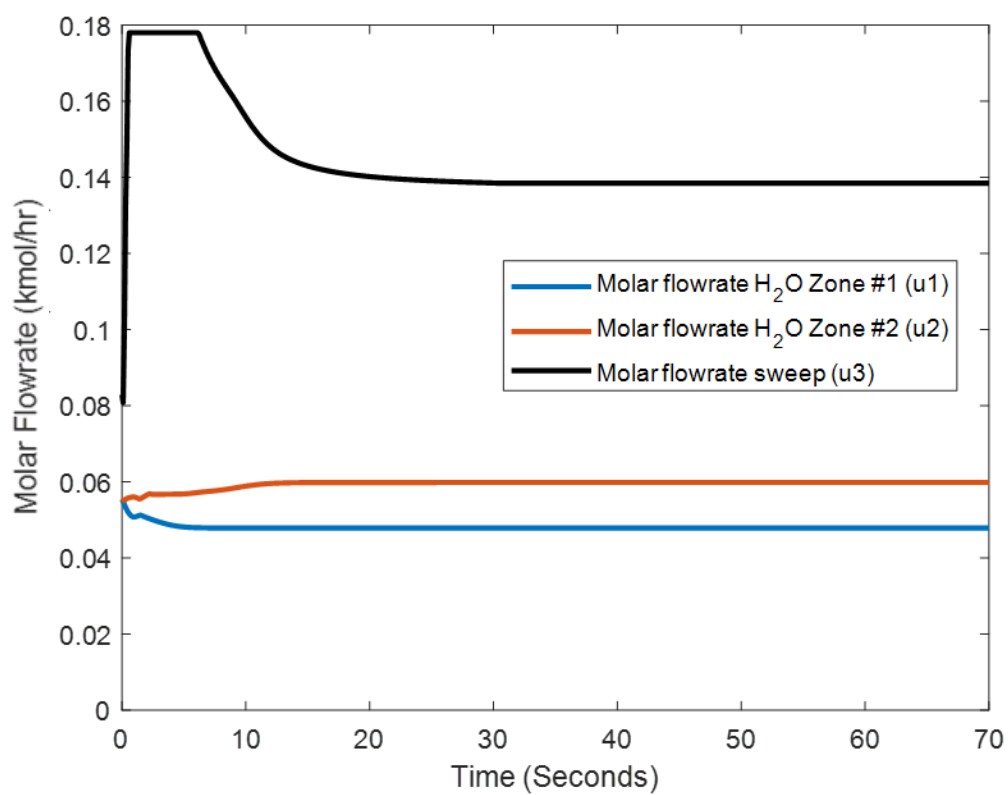


Figure 13. Quadratic Dynamic Matrix Control Input Results - Online connection to Aspen Model

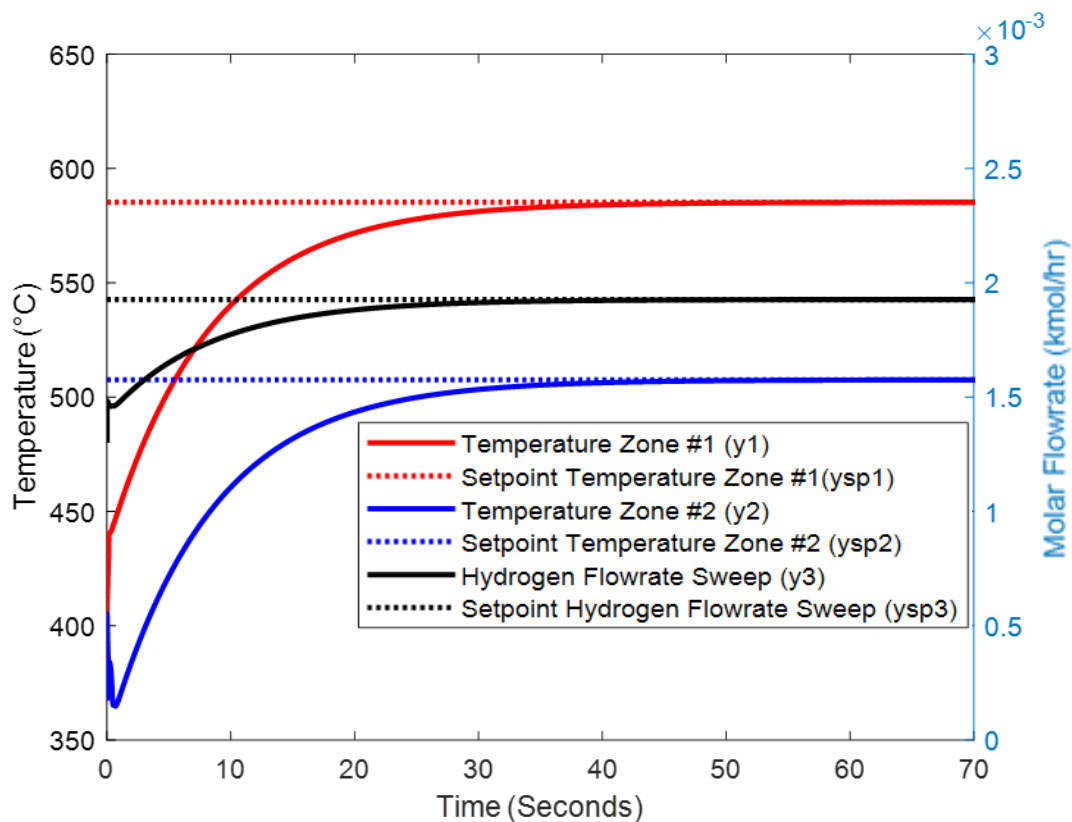


Figure 14. Quadratic Dynamic Matrix Control Output Results - Online Connection to Aspen Model

The QDMC was able to reach the desired setpoint in 60 seconds. The average computational time per control step was found to be of 0.31 seconds. With the computational time per control step being under the time each control action was taken, this control strategy was able to run online on the Aspen Custom PDE model.

5.3.2 BIO-CS cast as MPC

The second linear MPC control strategy implemented on the WGS membrane reactor was the BIO-CS. This controller can reach steady state in around 18 seconds and had a relatively high computational time per control step of 0.82s. As the computational time per control step was under one and no physical constraints are

violated, an online real-time control study was able to be completed on the first-principles Aspen model. The BIO-CS result can be seen in Figures 15 and 16.

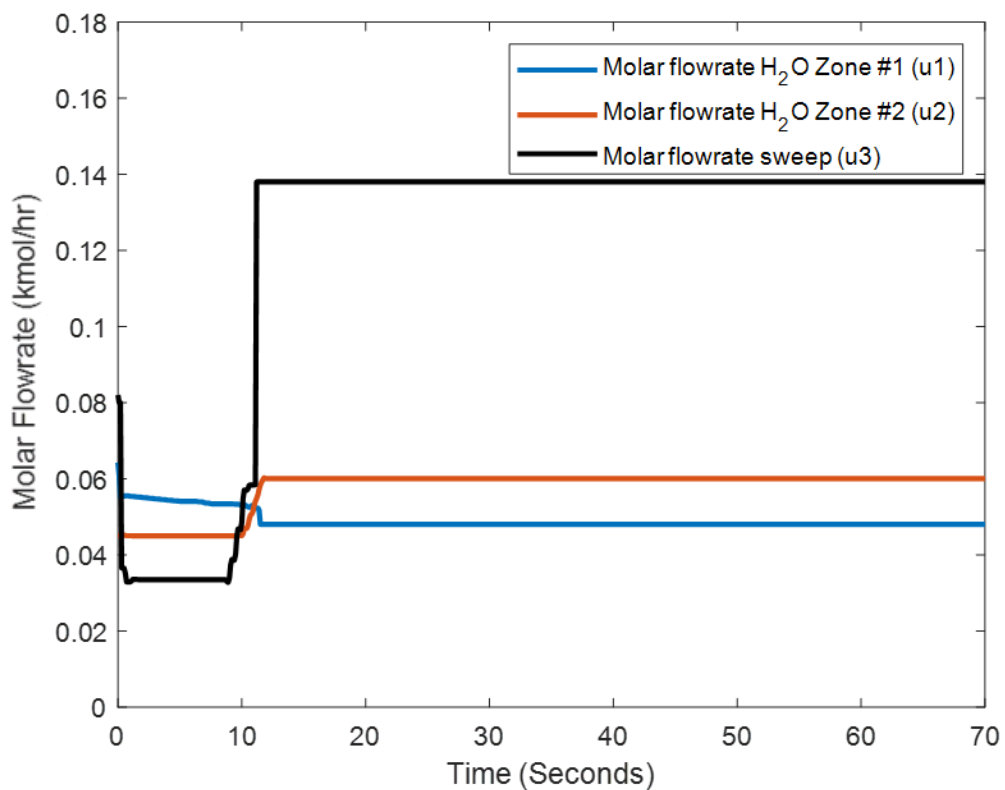


Figure 15. BIO-CS as MPC Control Input Results - Online Connection to Aspen Model

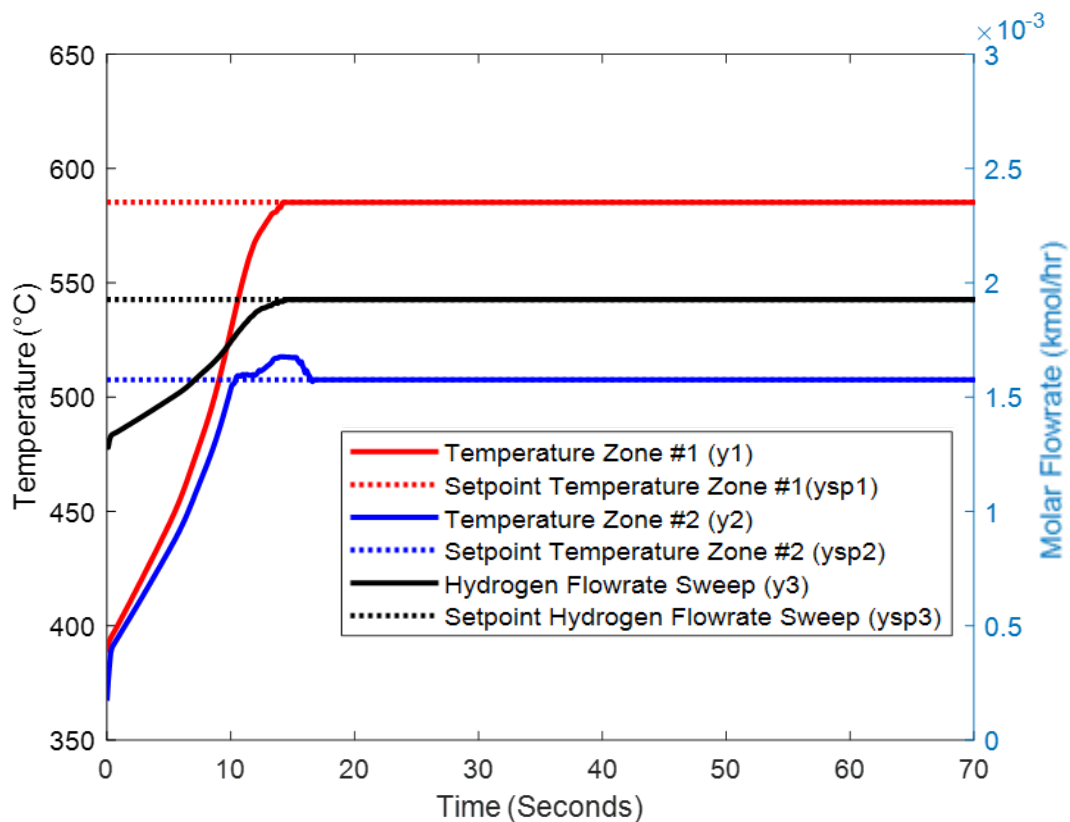


Figure 16. BIO-CS as MPC Control Output Results - Online Connection to Aspen Model

5.4 Implementation of Nonlinear Model Predictive Controllers on Aspen Model to Simulate Setpoint Change

Similar to the linear control studies, the goal for the nonlinear model predictive control strategy was to increase the outlet hydrogen concentration in the sweep stream by 15% while also making sure the temperatures of the outlet first reactive zone was of 585.24°C and the outlet second reactive zone was of 507.52°C.

5.4.1 NMPC

The nonlinear MPC applied to the WGS membrane reactor model was the NMPC. This controller utilized the NARX model to ensure a minimum plant-model mismatch. The NMPC is able to reach steady state the fastest at a time of 15 seconds, but had the highest computational time per control step being of 0.91s. As the computational time per control step was under 1, the controller can be implemented online and in real time with the Aspen PDE model. The NPMC result can be seen in Figures 17 and 18.

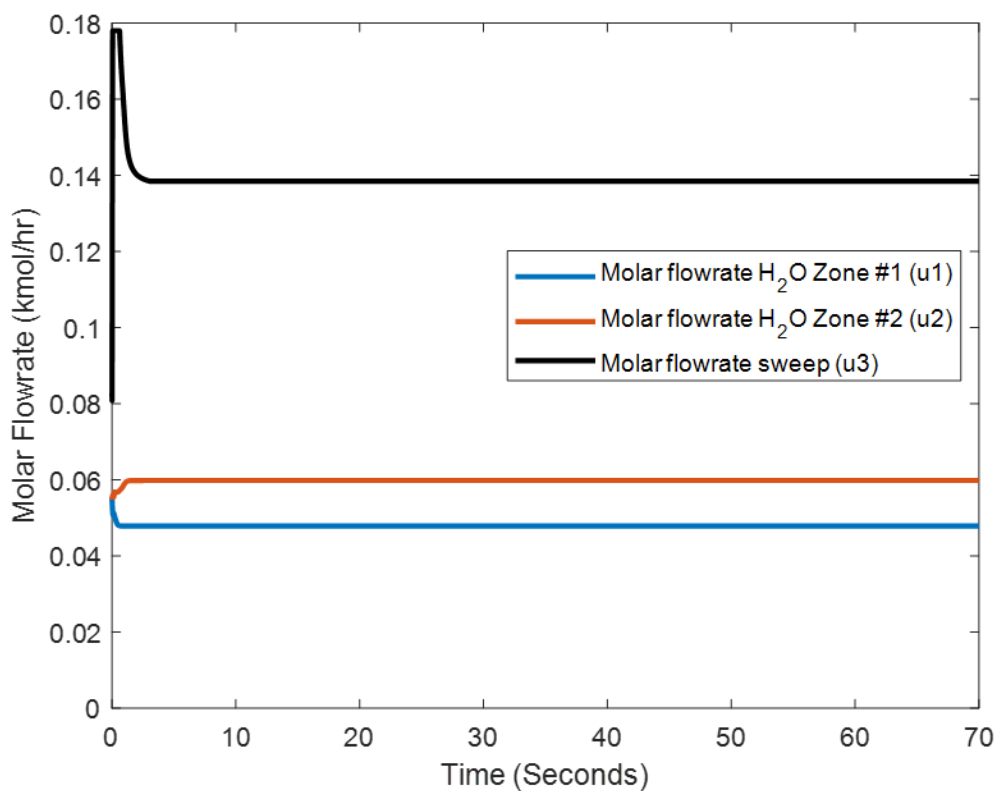


Figure 17. NMPC Control Input Results - Online Connection to Aspen Model

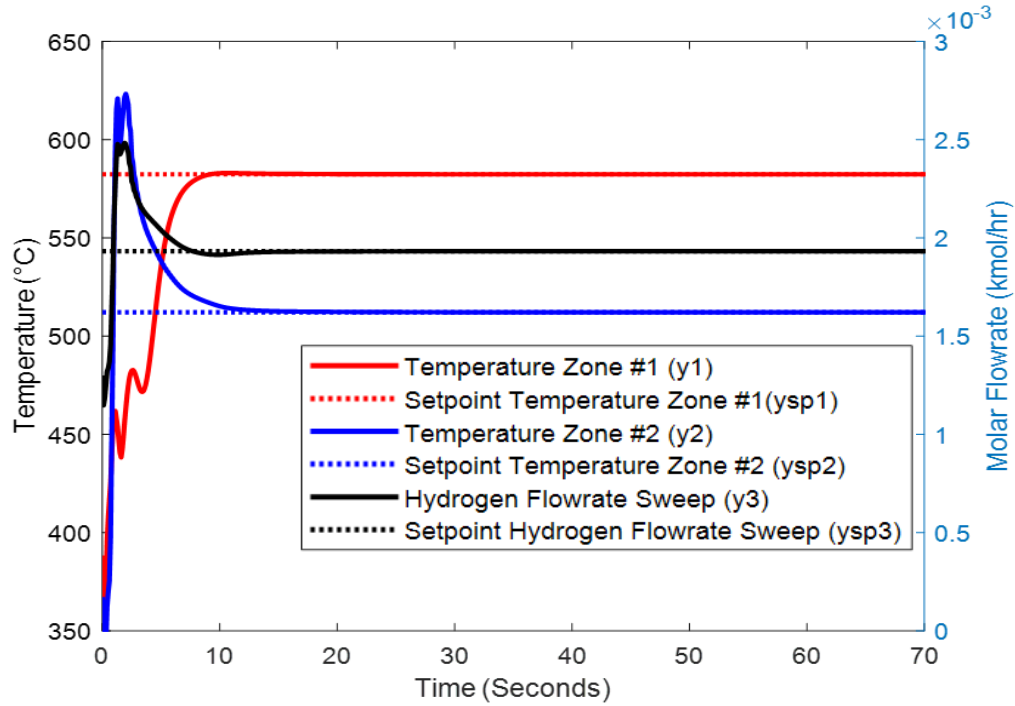


Figure 18. NMPC Control Output Results - Online Connection to Aspen Model

A comparison of the results between the control strategies implemented can be seen in Table 2, considering the average computational time, time to reach steady state and integrated square error (ISE) values for each controller.

Table 4. Control Implementation Performance Summary

Control Strategy	Control Model Used	Average computational time per control step	Time to reach steady state	Integrated Square Error y1 [-]	Integrated Square Error y2 [-]	Integrated Square Error y3 [-]
QDMC	ARX	0.31 seconds	60 seconds	9.47×10^6	9.83×10^6	1.05×10^{-5}
NMPC	NARX	0.97 seconds	15 seconds	7.99×10^5	3.92×10^5	8.02×10^{-6}
BIO-CS	ARX	0.85 seconds	18 seconds	2.02×10^6	6.15×10^5	1.98×10^{-6}

5.5 WGS Membrane Reactor Model Concentration and Temperature Profiles after Control Strategy Implementation

After the completion of the control strategies, an investigation was performed on the concentration and temperature profiles found within the Aspen model. The concentration profile from the NMPC control strategy can be seen in Figure 19 shows that the highest concentration of H_2 in the reactive section shifted further down the reactor to around 5cm when compared to 2-3 cm in the open loop case.

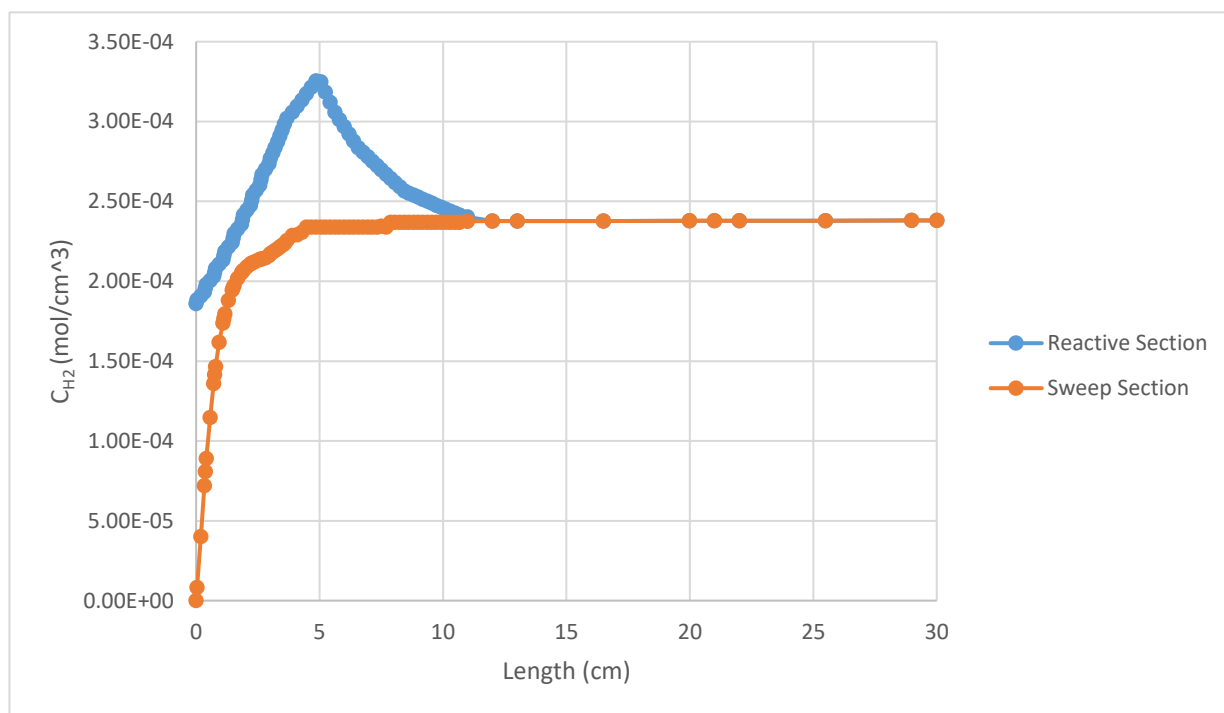


Figure 19. WGS Membrane Reactor Closed Loop Concentration Profiles from Aspen Model

Subsequently, the temperature profile of the reactive section of the reactor also changed from the open loop case. In Figure 20, the max temperature in the reactor is found at around 6-7cm, while in the open loop case the max temperature took place around 5cm.

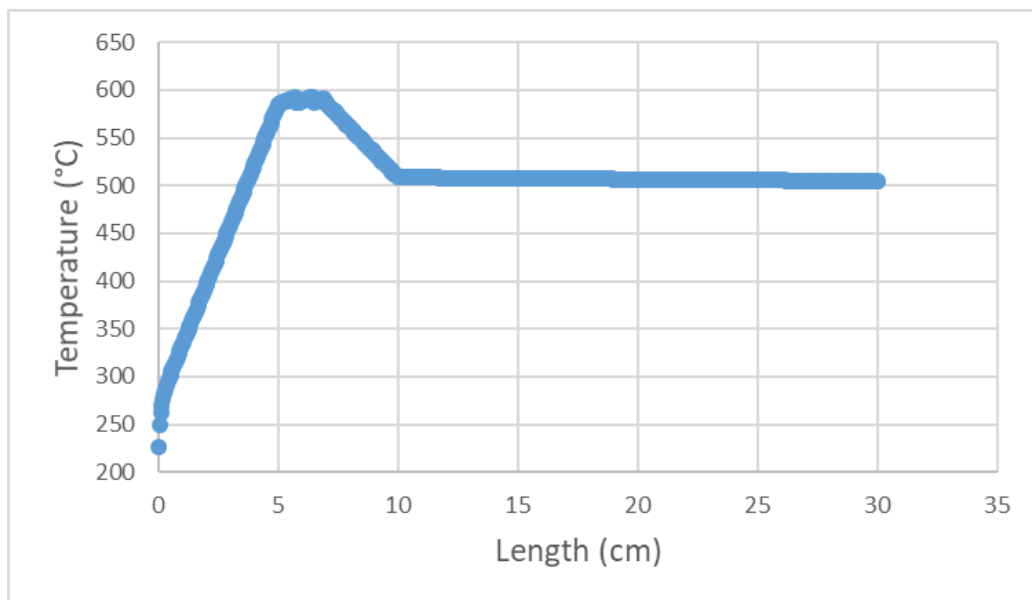


Figure 20. WGS Membrane Reactor Closed Loop Temperature Profiles from Aspen Model

6. Conclusions

A detailed and comprehensive nonisothermal, nonisobaric water-gas shift membrane reactor model was created in Aspen Custom Modeler V9 and validated through other similar models found in literature. Both linear and nonlinear model predictive control strategies were applied to the process to attempt to increase the concentration of the H_2 in the sweep gas by +15%. The model predictive control strategies that were applied to the system included: QDMC, NMPC, and BIO-CS.

Each of the three control strategies were able to reach the new steady state without violating any physical constraints and being able to run online in real time. All control strategies followed a similar path to reach the desired setpoint, with some variations. Such variations can be attributed to the difference in the solvers and types of models used to predict the control actions that would be implemented on the plant model.

QDMC had the fastest computational time of the three viable controllers with an average computational time per control action being of .31s but had the slowest time in achieving the desired setpoint taking 60 seconds. Also, QDMC utilized a linear ARX model to predict control actions, with the disturbance rejection term used to alleviate the plant model mismatch causing a longer time to reach steady state than if the strategy utilized the NARX model.

NMPC had the slowest computational time of the three viable controllers with an average computational time per control action being of 0.97s but had the fastest time in achieving the desired setpoint taking 15 seconds.

BIO-CS had an average computational time per control action of 0.85s and had the fast time in achieving the desired setpoint for a linear MPC taking 18 seconds. BIO-CS utilized a linear ARX model that is converted into a system of ordinary differential equations model to predict control actions, the disturbance rejection term used helped to alleviate the plant model mismatch causing a longer time to reach steady state than if the strategy utilized the NARX model.

The NMPC had an average computational time per control step that was close to one. If the control action is kept at 1 second, this control strategy may not be feasible in a higher dimensional case. QDMC would have no trouble being applied to a higher dimensional case and BIO-CS would have no trouble being used in a slightly higher dimensional case.

In conclusion, the online implementation of both linear and nonlinear MPC strategies on an Aspen Custom WGS membrane reactor was successful. The different control strategies showed a decrease in the time to transition to a desired steady state from 60 seconds using QDMC to 15 seconds using NMPC, while also decreasing the integrated square error for the systems outputs.

7. Future Recommendations

7.1 Change Solver used in BIO-CS to Non-Derivative-based Solver

In the current version of BIO-CS, the control strategy utilizes the DYNOPT solver to calculate the optimal control strategy. This solver requires a set of ordinary differential equations which is easy to calculate from a state-space model, but difficult if a NARX model is used. Along with the ability to use black box models, such as NARX, the possibility of the parallelization of BIO-CS would also be an interesting research direction.

7.2 Use In-House Optimizer to Decrease Computational Time Required for NMPC and BIO-CS

Most readily available optimizers have some background calculations that are used to help solve problems if the optimizer cannot find a solution. These extra calculations will increase the time needed to find the solution. With an in-house optimizer the backend computational time could be decreased.

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