

MODEL PREDICTIVE CONTROL OF A TUBULAR AMMONIA REACTOR-HEAT EXCHANGER SYSTEM WITH SQUARE AND NON-SQUARE CONTROL STRUCTURES USING SINGULAR VALUE DECOMPOSITION (SVD)

Part II: Application to an Ammonia Reactor-Heat Exchanger System

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ABSTRACT

In this paper, we present the application of a model predictive control (MPC) strategy to a tubular ammonia reactor-heat exchanger system based on the singular value decomposition (SVD) approach to computation of the control law. The SVD-based MPC controller was used to evaluate various 2×2 , 2×3 and structures under nominal, additive plant/model mismatch, and measurement noise. The closed-loop simulation results validated the previously reported outcome of the selection of the most promising 2×2 and 2×3 control structures, and rejection of the 3×3 control structures based on dynamic resilience analysis. The designed SVD-based MPC controllers performed better than a decentralized PI controller previously reported in the literature.

1 INTRODUCTION

Improved control and operation of an ammonia reactor system is an industrially important goal since the Haber process for production of ammonia is the major process in the manufacture of nitrogenous fertilizers - a vital input for modern agricultural farming.

Williams and Adeniyi (2018a) applied the dynamic resilience analysis technique for selection of the most promising control structures for a tubular ammonia reactor-heat exchanger system from the literature. This was undertaken as part of the task of advanced control design for the system such as model predictive control (MPC).

In a companion paper (Part I), the formulation of the MPC problem starting from a state-space model, derivation of the control law and its computation using the Singular Value Decomposition (SVD) was presented. In the present paper (Part II), the SVD-based MPC is applied to a series of previously selected control structures of the tubular ammonia reactor-heat exchanger system and assessed using closed-loop computer simulations.

An abridged version of this work which considered only 2×2 control structures was presented in Williams and Adeniyi (2018b). This current work expands on this to include 2×3 (non-square) and 3×3 (square) control structures, along with presentation of essential details that could not be included in the abridged paper. Comparisons of the performance of the SVD-based model predictive controllers with multi-loop PI

controllers previously reported in the literature are also presented.

2 THE AMMONIA TUBULAR-REACTOR HEAT EXCHANGER SYSTEM

A schematic diagram of the ammonia synthesis reactor-heat exchanger system under consideration as presented by Patnaik *et al.* (1980a,b) and Viswanadham *et al.*, 1979) is shown in Figure 1. The inlet gaseous mixture is split into three separate streams: (i) the main stream called the heat exchanger flow, $F_1(u_1)$; (ii) the second stream called the heat exchanger by pass flow, $F_2(u_2)$; and (iii) the third stream called the direct by pass flow, $F_3(u_3)$.

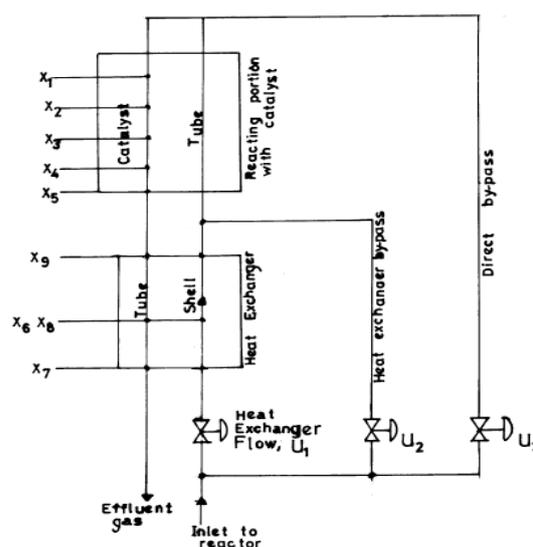


Figure 1: Schematic of ammonia synthesis reactor (Patnaik *et al.*, 1980a,b; Viswanadham *et al.*, 1979)

3 CONTROL STRUCTURES IDENTIFIED FROM DYNAMIC RESILIENCE ANALYSIS

Various control structures identified for the ammonia reactor-heat exchanger system using dynamic resilience analysis (Williams and Adeniyi, 2018a) which shall be considered in the SVD-based MPC design and closed-loop simulation evaluation are as follows:

- 2×2 control structures
 - (a) structure D i.e. control x_1 and x_5 with u_1 and u_2 .
 - (b) structure P i.e. control x_1 and x_9 with u_1 and u_2 .
 - (c) structure X i.e. control x_1 and x_5 with u_1 and u_3 .
 - (d) structure AR i.e. control x_1 and x_5 with u_2 and u_3 .
- 2×3 Control Structures.
 - (a) structure BL i.e. control x_1 and x_5 with u_1 , u_2 , and u_3 .
 - (b) structure BN i.e. control x_1 and x_9 with u_1 , u_2 , and u_3 .
 - (c) structure BQ i.e. control x_2 and x_5 with u_1 , u_2 , and u_3 .
 - (d) structure BU i.e. control x_3 and x_5 with u_1 , u_2 , and u_3 .
- 3×3 Control Structure: structure CL i.e. control x_1, x_4 and x_5 with the three control variables u_1, u_2 , and u_3 .

4 APPLICATION OF MPC-SVD DESIGN TO THE TUBULAR-AMMONIA REACTOR-HEAT EXCHANGER SYSTEM

The model predictive controller designs for the ammonia reactor-heat exchanger system is based on the SVD technique presented in the companion paper (Part I). We considered design and closed-loop simulation evaluation for a number of 2×2 , 2×3 and 3×3 control structures of the ammonia reactor system.

Preliminary designs/closed-loop simulations to assess the effect of design/tuning parameters on performance were first carried out for a 2×2 system using the control structure D, based on a perfect model assumption. The design and closed-loop simulations to determine the best control structures for the 2×2 , 2×3 and 3×3 systems under nominal and plant/model mismatch

conditions are then carried out. Following these, comparisons are made between the performance of the multivariable model predictive controller, and the decentralized (single-loop) PI controllers of Viswanadham *et al.*, 1979 in order to establish which one is superior.

5 RESULTS AND DISCUSSION

5.1 Preliminary Designs and Simulations

The initial design and closed-loop simulation evaluation of the model predictive controller to aid in proper selection of “fixed” tuning parameters was carried out for the ammonia reactor system with control structure D. After some trials, we chose a sampling time, $\tau = 0.4$, and a model horizon, $N = 80$. We chose the controller horizon, $q = 10$ to guarantee flexibility in the tuning of the controller. The following values of prediction horizon (P) and manipulated input blocking strategy were considered for the preliminary designs and closed-loop simulations:

1. $P = 10$, $k_q = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9$
2. $P = 30$, $k_q = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9$
3. $P = 20$, $k_q = 0, 2, 4, 6, 8, 10, 12, 14, 16, 18$
4. $P = 30$, $k_q = 0, 3, 6, 9, 12, 15, 18, 21, 24, 27$

Table 1 shows the results of the SVD analysis of the model predictive controller design (with control structure D) using various values of P and k_q given above.

This table shows the computed singular values (σ_i), the condition numbers (η_i), and the normalized performance ($\bar{\rho}_i$) when $k = 1, 2, K, i$ singular values are retained in the controller solution and others are discarded.

It is seen from Table 1 that the controller design based on this structure should be fairly robust as the η_{20} values lie between 6.90 to 44.5 for the four values of P and k_q shown. We also see that heavier blocking of the control input significantly reduces η_{20} , especially as the P/q ratio increases. This also suggests better robustness of the controller with heavier blocking of the control inputs. As expected, Table 1 shows that the closed-loop system performance (as measured by $\bar{\rho}_i$) improves (i.e. lower $\bar{\rho}_i$) as more singular values are retained in the controller solution.

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Table 1: Results of SVD analysis of model predictive controller design for various values of P , q , and k_q . (Ammonia reactor system system with control structure D)

S/N.	Set (a)			Set (b)		
	σ_i	η_i	$\bar{\rho}_i$	σ_i	η_i	$\bar{\rho}_i$
1	0.0138	1.0000	0.9939	0.0631	1.0000	0.9922
2	0.0135	1.0206	0.9889	0.0495	1.2747	0.3342
3	0.0134	1.0334	0.9885	0.0138	4.5572	0.3342
4	0.0132	1.0436	0.9784	0.0135	4.6589	0.3237
5	0.0131	1.0545	0.9741	0.0134	4.7103	0.3147
6	0.0130	1.0616	0.9445	0.0133	4.7504	0.3089
7	0.0129	1.0693	0.9134	0.0131	4.8022	0.3070
8	0.0129	1.0723	0.8364	0.0130	4.8441	0.3062
9	0.0128	1.0761	0.7911	0.0129	4.8806	0.3059
10	0.0128	1.0778	0.7865	0.0129	4.9058	0.3058
11	0.0082	1.6822	0.0410	0.0128	4.9214	0.3057
12	0.0042	3.3136	0.0284	0.0090	7.0311	0.0176
13	0.0029	4.8375	0.0091	0.0044	14.3507	0.0084
14	0.0023	6.0884	0.0060	0.0029	22.0965	0.0031
15	0.0019	7.1098	0.0024	0.0022	28.4590	0.0016
16	0.0017	7.9490	0.0015	0.0019	33.5525	0.0007
17	0.0016	8.6305	0.0005	0.0017	37.6394	0.0003
18	0.0015	9.1625	0.0002	0.0015	40.8300	0.0001
19	0.0014	9.5454	0.0000	0.0015	43.1370	0.0000
20	0.0014	9.7767	0.0000	0.0014	44.5376	0.0000
S/N.	Set (c)			Set (d)		
	σ_i	η_i	$\bar{\rho}_i$	σ_i	η_i	$\bar{\rho}_i$
1	0.0208	1.0000	0.9014	0.0270	1.0000	0.7857
2	0.0195	1.0646	0.8975	0.0244	1.1039	0.7809
3	0.0192	1.0794	0.8974	0.0238	1.1314	0.7804
4	0.0191	1.0887	0.8959	0.0236	1.1434	0.7794
5	0.0189	1.0967	0.8959	0.0234	1.1514	0.7794
6	0.0188	1.1037	0.8946	0.0233	1.1578	0.7789
7	0.0187	1.1098	0.8945	0.0232	1.1628	0.7789
8	0.0186	1.1143	0.8938	0.0231	1.1666	0.7787
9	0.0186	1.1173	0.8938	0.0231	1.1690	0.7787
10	0.0182	1.1416	0.7921	0.0223	1.2090	0.7146
11	0.0148	1.3994	0.0467	0.0193	1.3983	0.0537
12	0.0095	2.1762	0.0440	0.0148	1.8242	0.0537
13	0.0066	3.1473	0.0154	0.0108	2.4902	0.0184
14	0.0050	4.1150	0.0128	0.0084	3.2298	0.0168
15	0.0041	5.0300	0.0069	0.0068	3.9877	0.0091
16	0.0035	5.8755	0.0058	0.0057	4.7363	0.0082
17	0.0031	6.6370	0.0041	0.0050	5.4485	0.0058
18	0.0028	7.2898	0.0037	0.0044	6.0866	0.0055
19	0.0027	7.7983	0.0034	0.0041	6.6002	0.0050
20	0.0026	8.1237	0.0033	0.0039	6.9354	0.0049

Plots in Figure 2 show the closed-loop simulation performance of the model predictive controller in the regulation of temperatures x_1 and x_5 for a 5°C step change disturbance in the reactor feed temperature, with various numbers of singular values retained in the

controller solution, and different tuning parameters. The corresponding control inputs (u_1, u_2) are shown in Figures 3.

When the foregoing plots are closely examined, one is able to make the following observations:

1. For different numbers of singular values (2 or more) retained in the controller solution, fast regulation of temperatures x_1 and x_5 without offsets is obtained.
2. The performance (settling time, overshoots, etc.) of temperature x_5 seem not to be affected by the values of P and k_q considered. However, the performance of temperature x_1 is slightly affected by values of P and k_q used. From Figure 2, it appears that $P=10, q=10$ and $k_q=0,1,K,9$ give the best performance for variable x_1 using feedback control alone.
3. From the plots of the control inputs (u_1, u_2), it is clear that it is not desirable to retain many singular values in the controller solution because it results in large and sudden changes in the controller outputs which might not be realizable in practice. It was generally found that retaining only 5 or less singular values in the controller solution seem to provide a more gradual change in the controller output which may be more readily achieved in practice.

On the basis of the foregoing observations, the following may be recommended in the tuning of the model predictive controller for the ammonia reactor system:

1. With no blocking of the manipulated variable i.e. $k_q=0,1,2,K,9$, using $P=q=10$ gives the best closed-loop performance. However, if better robustness is desired, it seems one should use $P=30, q=10$, and $k_q=0,3,6,K,27$.
2. The number of singular values retained in the controller solution should lie between 2 and 5 in order for the controller to yield practically realizable control inputs.

5.2 Closed-loop Simulation of Different Control Structures

We now present the results of the model predictive controller design and closed-loop simulation for the ammonia reactor-heat exchanger system using different

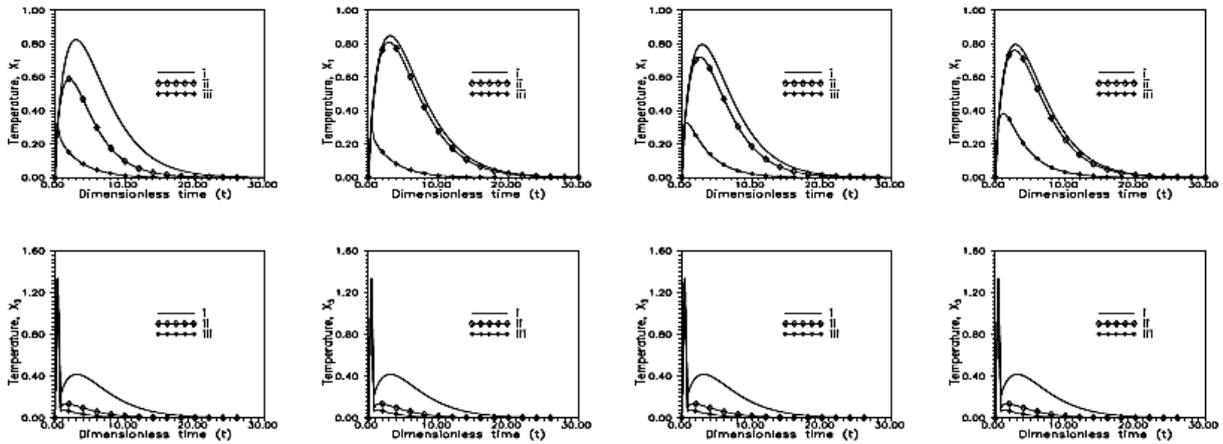


Figure 2: Closed-loop simulation responses of temperature x_1 (Top) and x_5 (Bottom) for a 5°C step change disturbance in reactor feed temperature under MPC. 1st, 2nd, 3rd & 4th column plots from left to right are for the tuning parameter sets (a), (b), (c) and (d), respectively. Legend: i, ii, iii for 2, 11, and 20 singular values retained in controller solution.

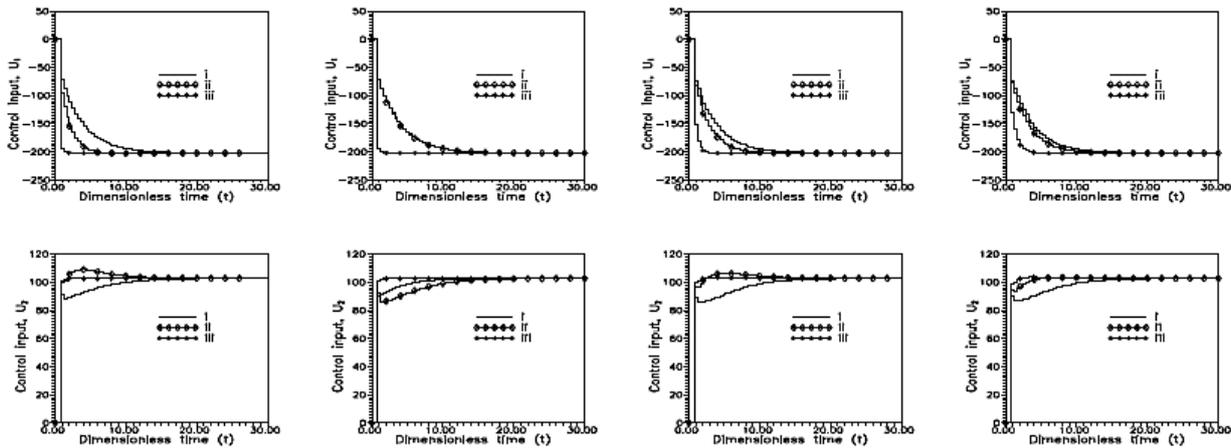


Figure 3: Manipulated control inputs: u_1 (Top) and u_2 (Bottom) for the response plots of Figure 2 1st, 2nd, 3rd & 4th column plots from left to right are for the tuning parameter sets (a), (b), (c) and (d), respectively. Legend: i, ii, iii for 2, 11, and 20 singular values retained in controller solution.

control structures. Closed-loop simulations were carried-out under nominal (perfect model assumptions) and model/plant mismatch conditions in the presence of significant noise in the temperature measurements. Model/plant mismatch conditions were created by assuming that the actual, linear plant matrices to be given by the following:

$$A_p = (1 + \Delta_e)A, \quad B_p = (1 + \Delta_e)B, \quad D_p = (1 + \Delta_e)D,$$

where A , B , and D are the linear model matrices employed in the model predictive controller designs.

The simulation results to be presented are for $\Delta_e = -0.9, 0$ and 0.9 in the case of the 2×2 , 2×3 ,

and 3×3 control structures with $\Delta_e = 0$ being the nominal case in which there is no model/plant mismatch. In all cases, temperature measurement noise was simulated by adding independent, zero-mean, normally distributed random numbers, each with a variance of 0.025 to the states x_1 to x_6 to produce the measured temperatures, two of which are fed back for control. The zero-mean, normally distributed random numbers were generated using a random number generator based on the algorithm presented in Forsythe *et al.* (1977). For the simulation results which follow, only feedback control was employed in the model predictive controller i.e. there

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is no feedforward of the measurable, reactor feed temperature disturbance. The following tuning parameters were used for all the simulations: $\tau = 0.4$, $N = 80$, $P = 10$, $q = 10$, and $k_q = 0, 1, 2, K, 9$.

5.2.1 2×2 Control Structures

The following 2×2 control structures were selected for controller design and closed-loop simulation testings (a) structure D i.e. control x_1 and x_5 with u_1 and u_2 , (b) structure P i.e. control x_1 and x_9 with u_1 and u_2 , (c) structure X i.e. control x_1 and x_5 with u_1 and u_3 , and (d) structure AR i.e. control x_1 and x_5 with u_2 and u_3 . Note that structures D and AR were identified as the best structures according to the dynamic resilience analysis earlier reported in Williams and Adeniyi (2018a) so we have included structures P and X only for the purpose of comparisons.

For a 5°C step change disturbance in reactor feed temperature, Figure 4 shows the closed-loop simulated responses of the five temperatures (x_1 to x_5) along the reactor length for the four control structures, with only four (4) singular values retained in the controller solution. The plots show the closed-loop responses (of x_1 to x_5) for the nominal and the two model/plant mismatch cases. The corresponding control inputs are shown in Figures 5.

When the plots of x_1 to x_5 are examined, we can see that on the whole, structure AR gives the best performance in terms of how well the variables are regulated about the origin, magnitude of steady-state offsets (where these occur), magnitude of control efforts, and sensitivity to model/plant mismatch. This is then followed by structure D, while it is difficult to rank the overall performance of structures P and X. This is because, structure X has better closed-loop responses (of x_1 to x_5) than structure P. However, structure X requires much larger magnitudes of control input u_1 (than for structure P), which may be impossible to implement practically.

Although the closed-loop responses (of x_1 to x_5) for structure X are clearly better than those of structure D, we have ranked those of the latter to be better based on the magnitudes of control inputs necessary to achieve the regulatory task. It is of course clear, that the closed-loop

responses (of x_1 to x_5) for structure D are, on the whole better than those of structure P since that of the latter exhibits large offsets in variables x_3, x_4 , and x_5 ; and also requires considerably larger control inputs (u_1 and u_2).

From the foregoing simulation results, we see that the closed-loop simulation results confirm the outcome of our earlier work for the selection of the most promising 2×2 control structures (Williams and Adeniyi, 2018a) based on dynamic resilience analysis i.e. structure AR is indeed the best followed by structure D.

5.2.2 2×3 Control Structures

The following control structures were selected for controller design and closed-loop simulation assessments: (a) structure BL i.e. control x_1 and x_5 with u_1, u_2 , and u_3 , (b) structure BN i.e. control x_1 and x_9 with u_1, u_2 , and u_3 , (c) structure BQ i.e. control x_2 and x_5 with u_1, u_2 , and u_3 , and (d) structure BU i.e. control x_3 and x_5 with u_1, u_2 , and u_3 . Again, it should be noted that structures BL and BQ were identified as the best structures according to the dynamic resilience analysis outcome reported in Williams and Adeniyi (2018a); we have included structures BN and BU only for the purpose of comparisons.

For a 5°C step change disturbance in reactor feed temperature, Figure 6 shows the closed-loop simulated responses of the five temperatures (x_1 to x_5) along the reactor length for the four control structures, with only four (4) singular values retained in the controller solution. The plots show the closed-loop responses (of x_1 to x_5) for the nominal, and the two model/plant mismatch cases. The plots of the corresponding control inputs u_1, u_2 , and u_3 are shown in Figure 7.

When the plots of x_1 to x_5 are examined, we can see that on the whole, structure BL gives the best performance in terms of how well the variables are regulated about the origin, magnitude of steady-state offsets (where these occur), magnitude of control efforts, and sensitivity to model/plant mismatch. This is.

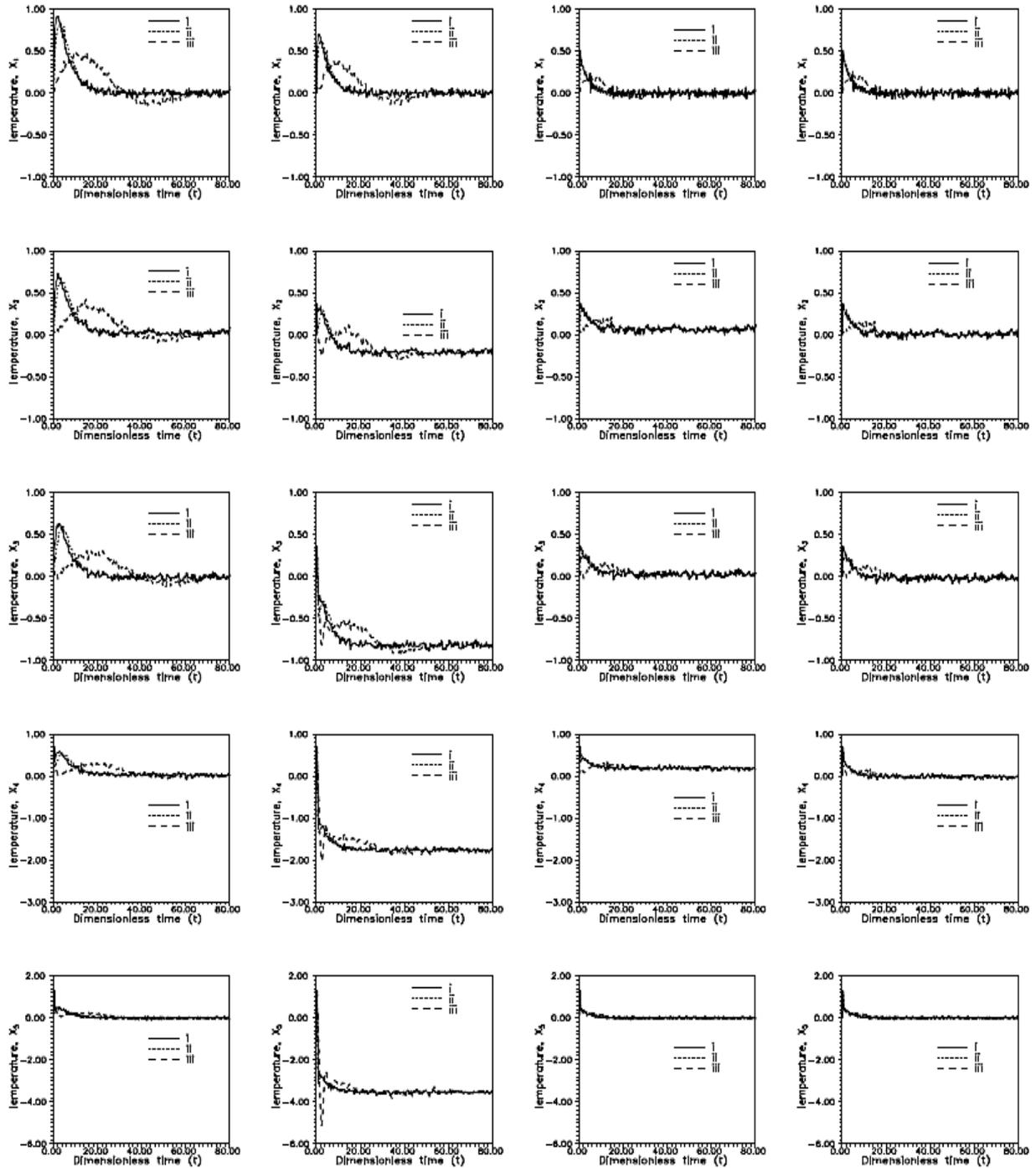


Figure 4: Closed-loop simulation responses of temperatures along the tubular reactor length (x_1 , x_2 , x_3 , x_4 & x_5 for a 5°C step change disturbance in reactor feed temperature under MPC with 4 singular values retained. 1st, 2nd, 3rd & 4th column plots from left to right: 2×2 control structures D, P, X, and AR, respectively. Legend: i, ii, iii for $\Delta_e = 0.9, 0, -0.9$, respectively.

then followed by structures BQ, BN and BU, in that order. Note the high sensitivity of structure BU especially for the model/plant mismatch case with $\Delta_e = -0.9$. This kind of high sensitivity was predicted by the dynamic resilience analysis and is clearly not desirable

for practical implementation purposes. It is for this reason that the performance of structure BN (even though it leads to offsets) was ranked better than that of structure BU

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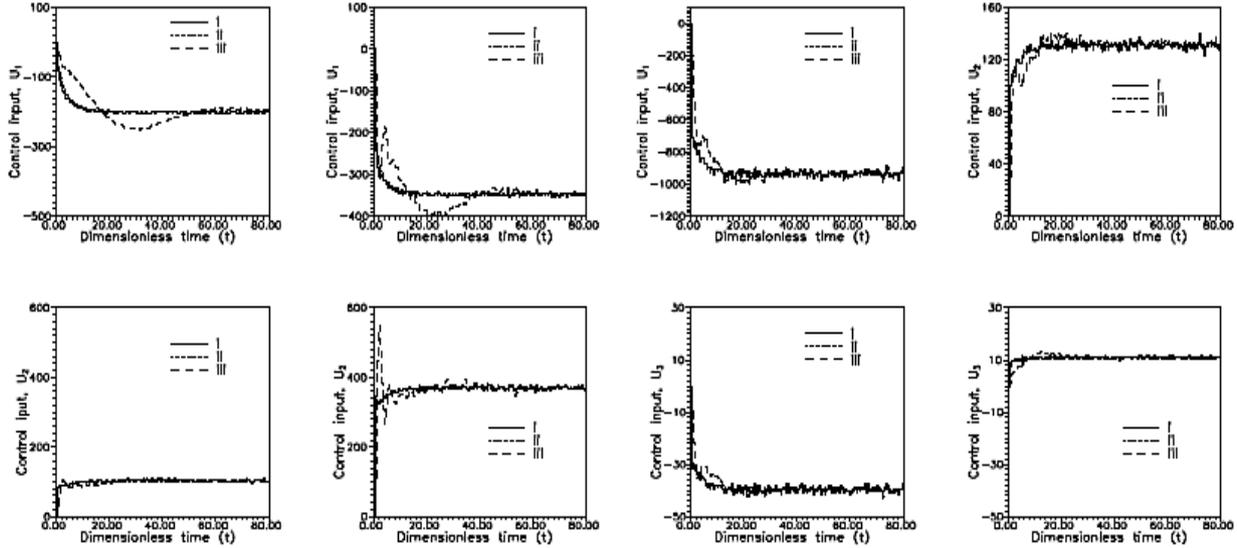


Figure 5: Control inputs for the response plots of Figure 4. 1st (u_1, u_2), 2nd (u_1, u_2), 3rd (u_1, u_3) & 4th (u_2, u_3) column plots from left to right: 2×2 control structures D, P, X, and AR, respectively. Legend: i, ii, iii for $\Delta_e = 0.9, 0, -0.9$, respectively.

Again, we see that the closed-loop simulation results also confirm the outcome of our earlier work for the selection of the most promising 2×3 control structures (Williams and Adeniyi, 2018a) based on dynamic resilience analysis. As expected from the results of dynamic resilience analysis, and physical reasoning, comparison of the closed-loop simulation responses and the control inputs for the 2×2 and the 2×3 control structures show the latter to be generally better.

5.2.3 3×3 Control structures

The results of dynamic resilience analysis reported in Williams and Adeniyi (2018a) indicated that only the 2×2 and 2×3 control structures can be used for practically useful controller designs, while the 3×3 would not lead to a useful controller design. To confirm this, we selected the best 3×3 structure i.e. structure CL, which is to control x_1, x_4 and x_5 with the three control variables u_1, u_2 , and u_3 , for control design and closed-loop simulation testing under nominal, and model/plant mismatch conditions.

For a 5°C step change disturbance in reactor feed temperature, Figure 8 shows the closed-loop simulated responses of temperatures x_1, x_2, x_3 and x_5 with only four (4) singular values retained in the controller solution. The plots show the closed-loop responses for

the nominal and the two model/plant mismatch cases. The corresponding control inputs are also shown in Figure 8. Without making any comments, these plots clearly demonstrate the point that this structure is not suitable for carrying out any practically useful control system design for the ammonia reactor system. This is also in consonance with the outcome of the dynamic resilience analysis of the 3×3 control structures earlier reported in Williams and Adeniyi (2018a)

5.3 Comparison with decentralized PI controllers

Figure 9 shows the comparisons of the closed-loop simulated responses of the model predictive controllers (designed with the 2×2 and 2×3 control structures AR and BL, respectively), and those of the two single-loop PI controllers of Viswanadham *et al.* (1979), which were extensively tuned for best performance using closed-loop simulations, based on the 2×2 control structure AR. These figures respectively show the closed-loop simulated responses of temperatures x_1 and x_5 following a 5°C step change disturbance in the reactor feed temperature under nominal (i.e. perfect model, no noise), measurement noise, and two cases of model/plant mismatch plus measurement noise conditions. The measurement noise and the two cases of model/plant mismatch were as previously described. The corresponding control inputs for the plots in Figure 9 are shown in Figure 10

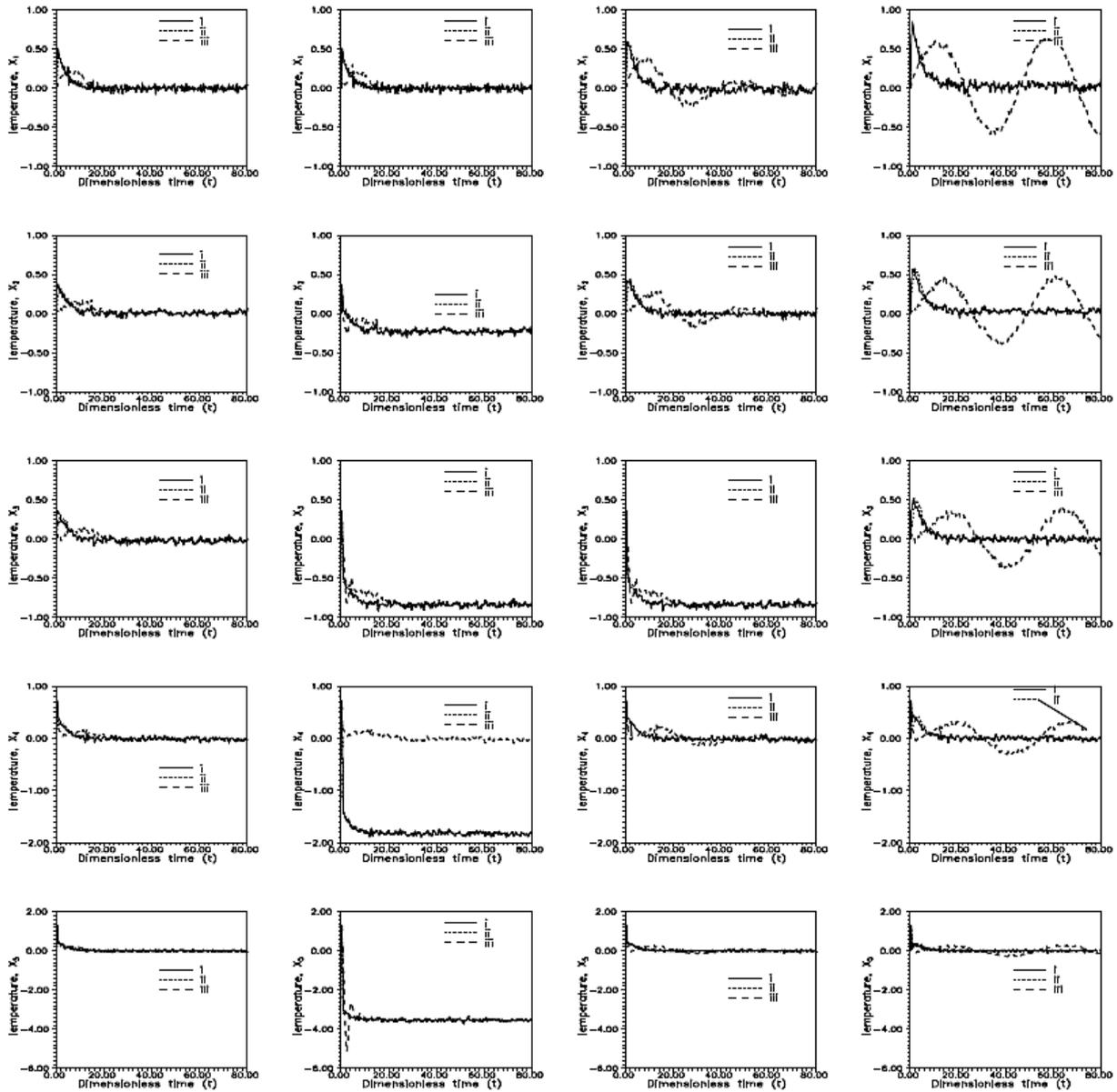


Figure 6: Closed-loop simulation responses of temperatures along the tubular reactor length (x_1, x_2, x_3, x_4 & x_5 for a 5°C step change disturbance in reactor feed temperature under MPC with 4 singular values retained. 1st, 2nd, 3rd & 4th column plots from left to right: are for 2×3 control structures BL, BN, BQ, and BU, respectively. Legend: i, ii, iii for $\Delta_e = 0.9, 0, -0.9$, respectively.

It can be seen from the foregoing figures that the model predictive controllers give better regulation of the temperatures x_1 and x_5 about the origin than the two single-loop PI controllers in all cases. Furthermore, the two single-loop PI controllers display larger sensitivity to the effect of measurement noise and model/plant mismatch as evident by the jagged movement of the control inputs. Such jagged movements are clearly undesirable as they will lead to rapid wear and tear of the final control element such as a control valve. Although the closed-loop responses of x_1 and x_5 are practically

the same for the 2×2 and 2×3 MPC, we can see that latter requires smaller inputs in u_2 and u_3 than the former, since u_1 is also moved. This clearly suggests, as previously predicted by dynamic resilience analysis (Williams and Adeniyi, 2018a), that the 2×3 structure is superior as it can handle disturbances of larger magnitudes (without saturation) than the 2×2 structure

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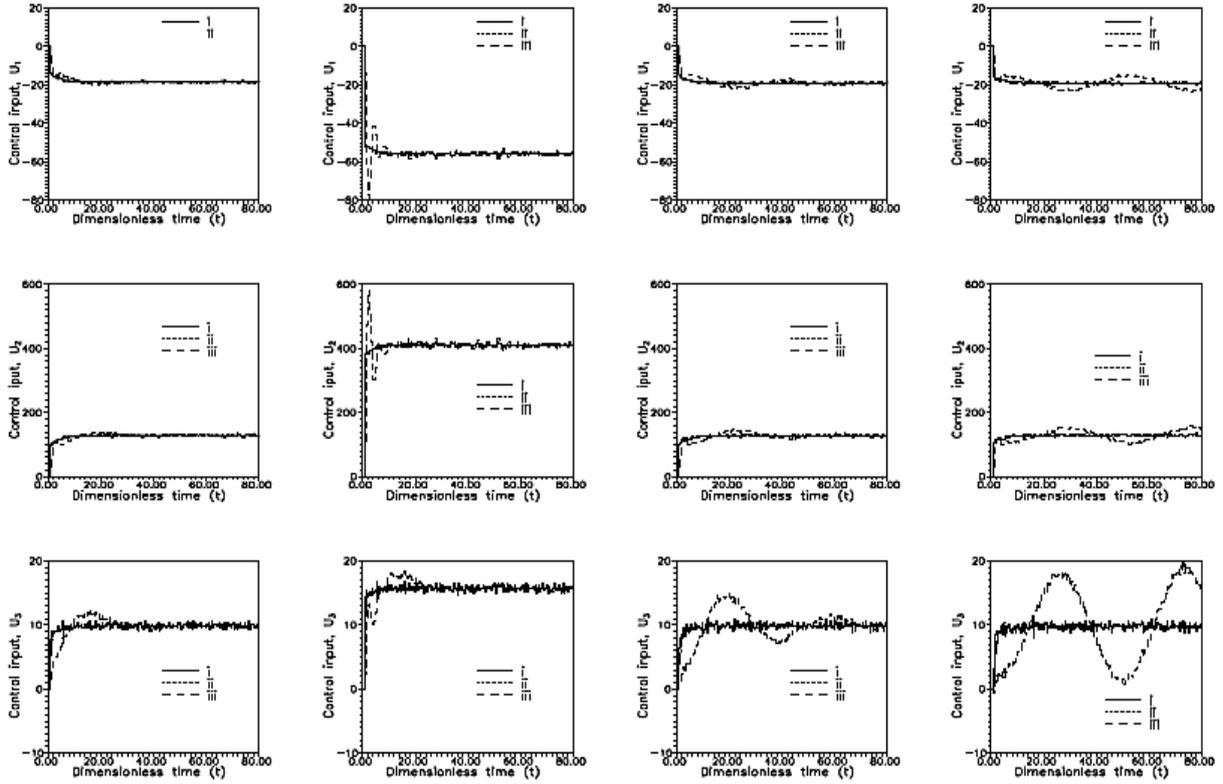


Figure 7: Control inputs (u_1, u_2, u_3) for the response plots of Figure 6. 1st, 2nd, 3rd & 4th column plots from left to right are for the 2×3 control structures BL, BN, BQ, and BU, respectively. Legend: i, ii, iii for $\Delta_e = 0.9, 0, -0.9$, respectively.

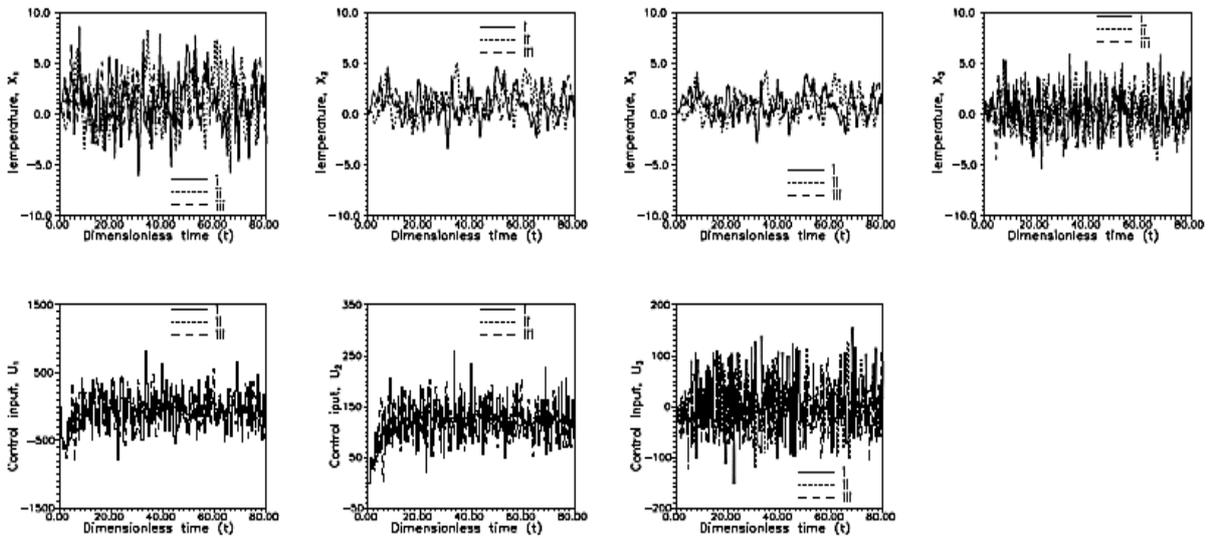


Figure 8: Top figures: Closed-loop simulation responses of temperatures x_1, x_2, x_3 , and x_5 for a 5°C step change disturbance in reactor feed temperature under MPC with 4 singular values retained. Bottom figures: corresponding control inputs, u_1, u_2, u_3 (for 3×3 structure CL). Legend: i, ii, iii for $\Delta_e = 0.1, 0, -0.1$, respectively. (Feedback configuration).

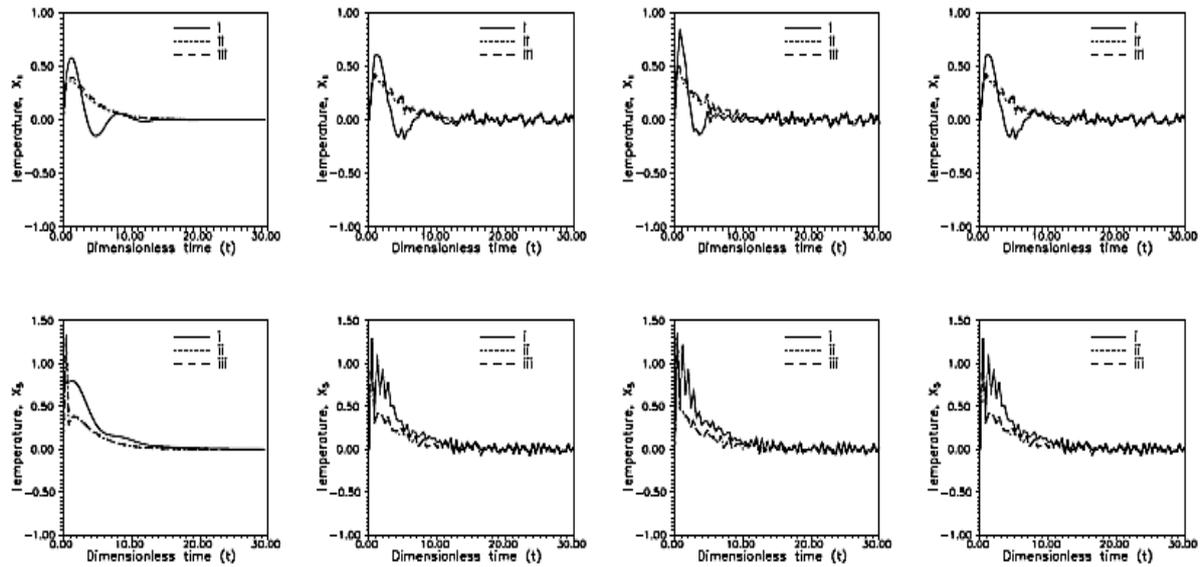


Figure 9: Comparisons of closed-loop simulation responses of temperatures for a 5° C step change disturbance in reactor feed temperature. Top: x_1 , Bottom: x_5 . 1st, 2nd, 3rd & 4th column plots from left to right are for the nominal, noise + $\Delta_e = 0$, noise + $\Delta_e = 0.9$, and noise + $\Delta_e = -0.9$, respectively. Legend: i, two single-loop PI controllers; ii, & iii 2×2 and 2×3 MPC, respectively.

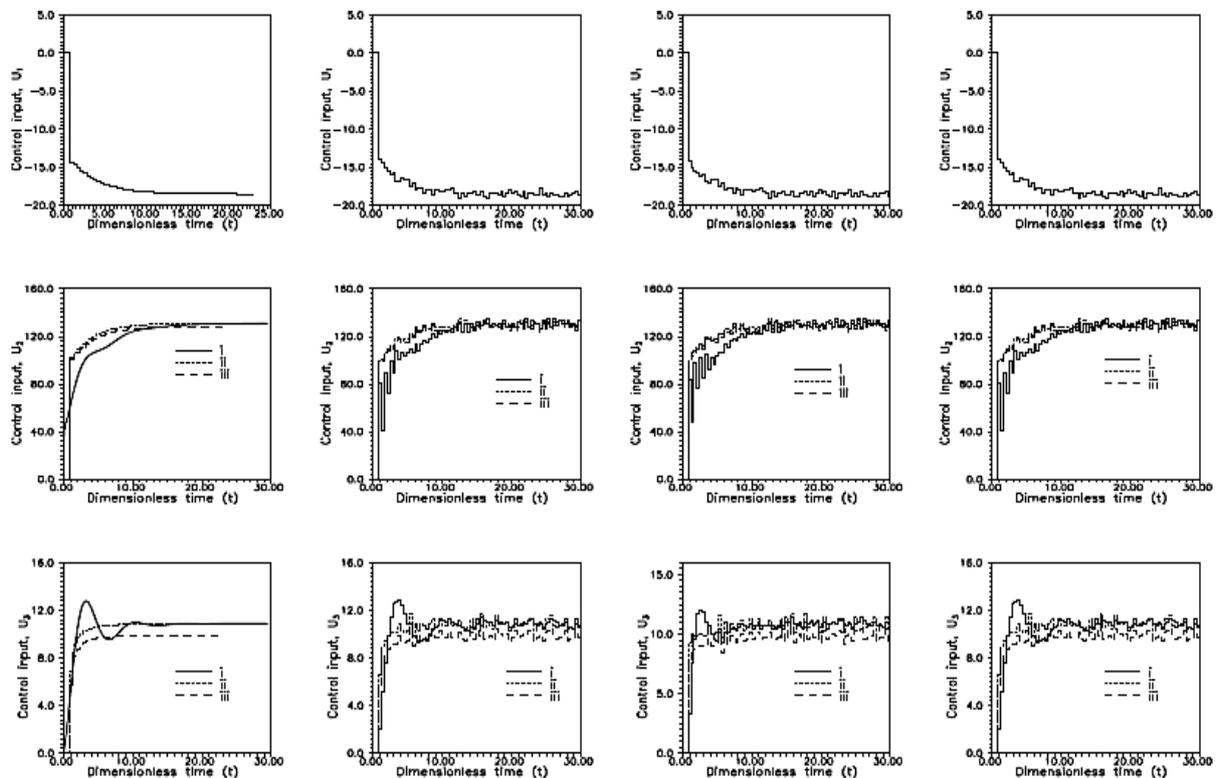


Figure 10: Control inputs for the 2×3 MPC with 4 singular values retained. Top: u_1 , Middle: u_2 , Bottom: u_3 . 1st, 2nd, 3rd & 4th column plots from left to right are for the nominal, noise + $\Delta_e = 0$, noise + $\Delta_e = 0.9$, and noise + $\Delta_e = -0.9$, respectively.

6 CONCLUSION

This paper presented the design of a model predictive

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controller for a tubular ammonia reactor-heat exchanger system using the singular value decomposition (SVD) approach to computation of the control law. The SVD-based model predictive controller was used to evaluate various 2×2 , 2×3 and 3×3 control structures under additive plant/model mismatch and measurement noise.

The closed-loop simulation results validated the previously reported outcome of the selection of the most promising 2×2 and 2×3 using dynamic resilience by the authors. Closed-loop simulations also confirmed that no practically useful controllers can be designed for the system using any of the 3×3 control structures. The designed SVD-based MPC controllers based on the selected 2×2 and 2×3 control structures performed better than a decentralized PI controller previously reported in the literature.

This method of using the SVD to compute the control law in model predictive control has also been successfully applied to another multivariable system under set point control. This shall be presented in a future paper

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