Design of Linear Controllers applied to an ethanol steam reformer for PEM fuel cell applications

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Abstract

This paper focuses on the design of a controller for a low temperature ethanol steam reformer for the production of hydrogen to feed a Protonic Exchange Membrane (PEM) fuel cell. It describes different control structures for the reformer and treats the control structure selection of this Multiple Input Multiple Output (MIMO) system. For each control structure, decentralised 2x2 controllers with Proportional Integral (PI) control actions in each control loop are implemented. The PI parameters are tuned and the performance of the different linear controllers is compared through simulation. For the evaluation of the proposed controllers, the dynamic response for different initial conditions and changes in the references is analysed, as well as the behaviour of the controlled system against disturbances.

1. Introduction

Bio-ethanol is considered a CO_2-neutral fuel, suited to diminish the use of the conventional fossil fuels based on petroleum and natural gas. In previous contributions [1-2] the authors reported results addressing the dynamic modelling and controllability analysis of a low temperature catalytic ethanol steam reformer for fuel cell hydrogen feeding. In this work, the design of linear controllers suitable for this ethanol reformer is reported and a comparative analysis between different controllers is performed through simulation. Given the high non linearity of the reformer, the tuning and simulation tasks of the work, based on a non linear model, are fundamental to validate the previous controllability analysis results, which were based on a linear model.

Up until now there have only been a few works that address the design and implementation of controllers for fuel reformers [3-4]. To the knowledge of the authors,

only [5 and 6] use bio-ethanol fuel. In [5] a thermal plasma reforming process is considered and in [6] different control structures are analysed but a final controller design is not proposed. Additionally, some process control researchers have developed systematic plant-wide control methodologies and applied them to chemical processes. Related to this, are remarkable the works made by the group of Basualdo, applied to several academic cases of study. In their last work reported [7] they applied a novel technique for the plant-wide control design to a bio-ethanol processor system for hydrogen production, followed by high and low-temperature shift reactors and preferential oxidation. [8] represents another significant contribution in this area. This paper studies two methodologies for control structure design using a commercial process simulator. Both methodologies were applied to an ethanol production plant with an energy integration technology known as split-feed. The proposed structures were tested to verify its performance and the most efficient for industrial applications was identified. However, these two works do not address the multiple input multiple output control problem of the reformer.

We believe that the design of controllers for ethanol steam reformers is a necessary step towards the integration of these systems to fuel cells. Specifically, we focus on simple linear controllers because they may be interesting for practical implementation in some applications. The control objectives considered are to keep hydrogen and CO flow rates at their reference values, oscillating around the nominal conditions. This nominal operating point maximises hydrogen yield and minimizes CO production, which is necessary to prevent CO poisoning of PEM fuel cells.

Our ethanol reformer operates in three separate stages: ethanol dehydrogenation to acetaldehyde and hydrogen, acetaldehyde steam reforming and water gas shift reaction. Additional purification units required to obtain the CO level adequate to the standard

PEM fuel cells have not been included in this study. The authors already modelled the reformer by using a one-dimensional, pseudo-homogeneous model based on mass and energy balances [1]. Based on the controllability analysis made in [2], that permitted to select the best control structures, only five of them are considered in this work in the search of the best controllers.

2. System and model description

The reformer studied comprises three stages: ethanol dehydrogenation to acetaldehyde and hydrogen over SnO_2 followed by acetaldehyde steam reforming over Co(Fe)/ZnO catalyst and water gas shift reaction. Kinetic data have been obtained under different experimental conditions and a dynamic model has been developed for a tubular reformer loaded with catalytic monoliths for the production of the hydrogen required to feed a PEMFC. The mathematical model is based on the mass balance and the energy balance. The numerical solution of the partial differential equations was accomplished by its transformation into an ODE- system by discretization of the spatial derivative. To this end, backward finite differences have been used for the different stages of the reforming unit with 15 discretization points in each stage. The resulting 285 order ODE equations were solved by an algorithm implemented in MATLAB^{TM} (ODE45 Dormand-Prince). Additional details regarding the mathematical model can be found in [2].

3. Control Structures

The reformer is a MIMO system that has multiple inputs (possible manipulated variables) and multiple outputs (variables of interest). As explained in [2] the flow rates

of ethanol and water at the reactor entrance (F_{C2H5OH}, F_{H2O}), the temperature of the entering mixture ($T_{gas,e}$), and the temperatures of the furnaces of the three reforming stages ($T_{F,S1}$, $T_{F,S2}$, $T_{F,S3}$) have been considered as inputs. As outputs to be controlled we have considered the flow rates of H_2 and CO (F_{H2} and F_{CO}) at the output of the reformer. In order to carry out the controllability study based on a linear model, different control indices were calculated in a previous work [2], which were used to predict the degree of directionality and the level of interactions in the system. These indices were calculated in steady state and in frequency domain. The controllability indices applied were the Morari Resiliency Index (MRI), the Relative Gain Array (RGA) and the Condition Number (CN).

- MRI is the minimal singular value of the open-loop transfer function, which stands for a specific input and output direction. The control system that presents large MRI is preferred. Large MRI values indicate that the process can handle disturbances without saturation of the manipulated variables [9].

- RGA is calculated from the gain array (G) according to the following expression [10]:

$$RGA(G) = G \times (G)^{-T}$$

where $\times$ is the Hadamard product and T denotes the transpose of the corresponding matrix. RGA indicates the preferable variable pairings in a decentralized control system based on interaction considerations and also provides information about integral controllability, integrity, and robustness with respect to modelling errors and input uncertainty.

- CN of the transfer function matrix is the ratio between the maximum and minimum singular values:

$$\gamma(G) = \frac{\bar{\sigma}(G)}{\underline{\sigma}(G)} \qquad (2)$$

where $\overline{\sigma}(G)$ is the maximum singular value and $\underline{\sigma}(G)$ the minimum singular value of the transfer function matrix. Small CN (lower than 10 in scaled systems), indicates a well controllable process [10].

Five different 2x2 control structures were selected as the most promising ones for the control of F_{H2} and F_{CO}. These structures are defined in Table 1. The five control structures consist of a decentralised control where only two inputs are chosen as manipulated inputs among the five possible and each manipulated variable is paired with one controlled variable; for example, Structure 1 corresponds to the manipulation of F_{C2H5OH} for the control of F_{H2}, and the manipulation of F_{H2O} for the control of F_{CO}. For all the structures, the controllers that have been used in each one of the control loops are PI controllers.

In order to obtain a versatile system able to adapt its production to the changing operating conditions of a fuel cell, the controller must control the flow of the final products, F_{CO} and F_{H2}, to a time varying reference value. The reference tracking is therefore the main objective of the controller. Anyway, the analysis of the controlled system is based on reference changes but also on disturbance rejection. For this reason we have studied the behaviour of the controllers introducing changes in the non-manipulated input variables to evaluate if the controller is robust against these disturbances. In some cases, the control system is evaluated at different operating points. In the dynamic response a pure delay of approximately 11 s is observed under the nominal operation condition defined in Table 2. This will have important implications in the design of the automatic control device for an integrated reformer and fuel cell system.

Control specifications

Since the reformer is aimed to the production of hydrogen for PEM fuel cell applications, the main variables to be controlled are the hydrogen flowrate and the CO flowrate. In this work the equipment connected to the reformer is not considered .The idea is to make a comparative analysis of the ability of different controllers of the H_2 and CO flowrates to track references and reject disturbances.

There are several considerations to take into account in assessing a controller's response to a change of reference or disturbance. In this work we have considered mainly the following:

• The controlled variable should reach its desired value as quickly as possible.
• The controlled variable should not be too oscillatory or have strong peaks.
• The manipulated variable should not be subjected to major changes, as they can affect other parts of the process.

4. Simulation results

In this section the response of the system controlled by the different control structures is shown. Simulations are done with the non-linear model of the ethanol reformer. In Table 3 the tuning parameters selected for each structure can be seen. Two tuning methods have been adopted: Ziegler-Nichols (Z-N) and Trial and Error (T-E). The trial and error method is used when the Z-N tuning parameters present important limitations in terms of control and stability. The Z-N is an industry-friendly method; the tuning of the parameters was made according to the theory developed in [11]. Specifically, the method of the process reaction curve was performed for all the structures. But due to the

high non-linearity of the system, in some cases, the Z-N tuning method results in a set of parameters that can be improved by trial and error. Since we are dealing with PI controllers, to tune the controllers parameters properly by trial and error through simulation is a possible task.

Structure 1

In Figure 1 we can see the controlled variables (F_{H2} and F_{CO}) for the following reference tracking problem: 10% increase in the CO reference and 10% increase in the H_2 reference at t = 50s and t = 400s, respectively. The initial operating point is set at the nominal operating conditions. Both controlled variables are brought at their reference values without important peaks and oscillations in approximately 200s; the response time cannot be reduced significantly changing the controller parameters. Figure 2 shows the time response of the manipulated variables corresponding to the same simulation scenario than Figure 1. Through these simulations we see that a 17% increase in the flow rate of ethanol is necessary to produce a 10% increase in the controlled variables (F_{H2}). In addition a 6% decrease in the flow rate of water is necessary to produce a 10% increase in the controlled variables (F_{CO}). With these values we can consider that the control effort under these conditions is reasonable in both loops, although from the results we can conclude that the first loop is the one that requires a larger effort to control the system.

Structure 2

As indicated in Table 3, in this structure the parameters of the controller have been tuned with the T-E (trial and error) method. In Figure 3, the controlled variables are plotted for the following simulation scenario: 1% increase in the CO reference and 1%

increase in the H_2 reference at t = 500s and t = 7200s, respectively. The reference tracking is achieved with proper profiles in about 2000 seconds. Larger setpoint changes were not possible without an important enlargement of the settling time.

The control effort corresponding to these setpoint changes (not shown) is the following: 1% increase in the controlled output (F_{C2H5OH}) is necessary to produce an 8% increase in the system output (F_{H2}). In addition a 1% increase in the controlled output ($T_{F;S2}$) is necessary to produce a 1% increase in the system output (F_{CO}). With these values we can consider that the control effort under these conditions is reasonable in both loops, although the first control loop requires more effort than the second control loop.

Structure 3

Figure 4 shows the molar flow rates of H_2 and CO under the following conditions: 5% increase in the H_2 reference and 10% in the reference of CO at t= 4000s and t = 50s, respectively. The outputs present an acceptable performance, however when the reference of CO changes the output has a greater overshoot. This may seem logical because the increase is double than that in the other reference value. The response time is approximately double than the response time with structure 1.

In this case, the controller must produce a 9.8% increase in the flow of water to produce a 5% increase in the controlled output (F_{H2}), and an increase of 2% in the $T_{F;S2}$ produces an increase of 10% in the molar flow rate of CO (F_{co}).

Structure 4

This structure was the worst of all the structures considered regarding the behaviour of the output of molar flows of H_2 and CO facing 1% increase in the CO reference and 1% in the reference of H_2 at = 400s and t = 15000s, respectively. Simulation results showed

that the controlled response took an extremely long period of time to reach its desired value, even with setpoint changes of only 1%.

Looking at the manipulated variable it could be seen that a 21% increase in the gas temperature entrance ($T_{gas;e}$) is necessary to produce a 1% increase in the controlled output or controled variable (F_{H2}), whereas a 2% decrease at furnace temperature ($T_{F,S2}$) in the stage 2 is necessary to produce a 1% increase in the controlled output (F_{H2}) . This disequilibrium between the input and output percentage changes is another bad characteristic of structure 4.

Structure 5

In this case the simulation corresponds to the following variation: 1% increase in the CO molar flow reference and 1% in the reference of H_2 molar flow at = 500s and t = 12000s, respectively. Also we can see that the response time is extremely large like in the structure 4; for this reason the control with this structure and under this scenario (variation in the input reference and control parameters) is non viable.

In the simulation we can see that the controller should produce a 5% increase in the $T_{F,S1}$ to produce a 1% increase in the controlled output (F_{H2}). And the controller should produce a 1% increase in the $T_{F;S2}$ to produce a 1% increase in the controlled output (F_{CO}). Then we can conclude that the control effort under these conditions is suitable for both control loops, however, the first loop needs a larger effort.

5. Analysis of results

Structure 1: Since structure 1 has the best performance another robustness test is done for this structure. It consists on the change of the operating conditions. The simulations

performed are 10% setpoint changes in both controlled variables (the same scenario of Figure 1) but from different operating points. The operation points are:

- OP_1 (ΔF_{C2H5OH}): 10% ethanol input increase while keeping the other 5 inputs constant
- OP_2 (ΔF_{H2O}): 10% water input increase while keeping the other 5 inputs constant
- OP_3 ($\Delta T_{gas,e}$): 10% furnace temperature input increase in the gas entrance while keeping the other 5 inputs constant
- OP_4 ($\Delta T_{F,S2}$): 10% furnace temperature input increase in the stage 2 while keeping the other 5 inputs constant

From the simulations carried out to evaluate the performance of the controller under different operating conditions, we conclude that the performance of the controller is similar regarding all tested points of operation, proving the robustness of the controller under these changes. However, some operating points are more favourable for the performance of the controller, such as OP_2, which has a lower overshoot to changes in the references. All this can be seen in figures 5 and 6 where we see the controlled variables facing setpoint changes in both loops. It can be seen that the controlled system is quite robust as it behaves in a similar way in all cases.

In order to analyze the behaviour of the controlled system against disturbances we make changes in the manipulated variables; the results are the following:

Structure 2: F_{H2O}, $T_{gas,e}$, $T_{F,S1}$ and $T_{F,S3}$ are changed with steps of 2% at different times. The influence of $T_{F,S3}$ is much larger than the influence of the other perturbations but for all disturbances the control system is able to reject their effect. It can also be seen that $T_{F,S3}$ has a larger effect on H_2 flow rate than on CO flow rate.

Structure 3: F_{C2H5OH}, $T_{gas,e}$, $T_{F,S1}$, $T_{F,S3}$ are changed. The disturbances are implemented by steps of 2% at different times. In this case the influence of $T_{F,S2}$ is similar than the influence of $T_{F,S3}$. We can consider that the performance of the controller under the disturbances in the non-manipulated inputs is adequate. As we see in structure 2, when we make changes in temperature the flow rate of H_2 is more affected than the flow rate of CO.

Structure 4: F_{C2H5OH}, F_{H20}, $T_{F,S1}$, $T_{F,S2}$ are changed. The steps are made using increases of 10% in the F_{C2H5OH}, F_{H20} manipulated variables and a 5% increase in the temperatures ($T_{F,S1}$, $T_{F,S2}$). All the variables have the same effect on the reactor outputs. Under this perturbation in the non-manipulated inputs the controller has a good performance. The controller is robust under perturbation in the manipulated variables.

Structure 5: F_{C2H5OH}, T_{H2O}, $T_{F,S1}$, $T_{F,S3}$ are changed. The controller has a good performance under these perturbations in the input variables. As we conclude in structures 2 and 3, when we make changes in temperature the flow rate of H_2 is more affected than the flow rate of CO.

6. Conclusions

In this paper we were able to control a low temperature ethanol steam reformer by linear controllers. The linear controller must keep the flow of F_{H2} and F_{CO} to its reference value, which changes with time in order to adapt the hydrogen production to the fuel cell demand. Therefore, setpoint tracking is the main objective of the controller. However, disturbance rejection has also been evaluated. The linear controllers analysed are based on five different control structures (pairs of manipulated variables) and consist of two control loops with a PI control law. The great non-linearity of the system and the interaction between loops has made impossible to give the same treatment for the

analysis of the different structures. Because of that, the tuning methods are not the same and the simulation scenarios are not the same. But some general characteristics of the different structures can be obtained. When we compare the behaviour of different controllers we can conclude that the time response is different: when we use structure 1, where both manipulated variables are flows, the response is much faster than in the other cases. For example, in structure 2 the response spends more than 2000s to reach its final value while on the other hand when we make changes in structure 1, the controller variable spends 200s to reach the final value. The worst case was seen in structure 4 where response times were at least an order of magnitude higher than the other structures. From structures 2, 3 and 5, the structure 3 has the faster response; similar to structure 1. This conclusion is very significant in the implementation of the controller, emphasising the superiority of structure 1 according to the criterion of time response. In all the structures the responses don't have oscillations. Therefore, we cannot say that a structure will be better or worse than the other evaluating this consideration.

The control structures are subjected to different changes in the references. The structures 1 and 2 support changes of 10% in both loops, having the responses appropriate dynamics, what cannot be said for the other pairs. On the other hand, the rest of the control structures are subjected to changes of 5%, 2% and 1%, because larger setpoint changes were not possible to control.

When analysing the behaviour of the controlled system under changes in inputs that are not used as control variables, we did not see important differences between structures. We can generally conclude that all structures showed a good rejection of non-manipulated inputs disturbances.

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Nomenclature

t	time (min)
T	temperature (K)
T_F	furnace temperature (K)
OP_n	operating point

Subscripts

e	reactor input
out	reactor output
gas	gas
C2H5OH	relative to ethanol
H2O	relative to water
C2H4O	relative to acetaldehyde
H2	relative to hydrogen
CO	relative to carbon monoxide

O2 relative to oxygen

S1 stage 1

S2 stage 2

S3 stage 3

Greek letters

Δ increment

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Figures

Fig. 1 F_{H2} and F_{CO} curves for 10% set point changes at t=50s and t=400s.

Fig. 2 Controller outputs for 10% set point changes at t=50s and t=400s.

Fig. 3 F_{H2} and F_{CO} curves for 1% setpoint changes at t=500s and t=7200s.

Fig. 4 F_{H2} and F_{CO} curves for 5% and 10% setpoint changes at t=4000s and t=50s, respectively.

Fig. 5 Output of the molar flow rate of H_2 with 10% setpoint changes at t = 50s and t = 400s.

Fig. 6 Output of the molar flow rate of CO with 10% setpoint changes at t = 50s and t = 400s.

Tables

	Loop 1	Loop 2
Structure 1	$F_{C2H5OH} \rightarrow F_{H2}$	$F_{H2O} \rightarrow F_{CO}$
Structure 2	$F_{C2H5OH} \rightarrow F_{H2}$	$T_{F,S2} \rightarrow F_{CO}$
Structure 3	$F_{H2O} \rightarrow F_{H2}$	$T_{F,S2} \rightarrow F_{CO}$
Structure 4	$T_{gas,e} \rightarrow F_{H2}$	$T_{F,S2} \rightarrow F_{CO}$
Structure 5	$T_{F,S1} \rightarrow F_{H2}$	$T_{FS2} \rightarrow F_{CO}$

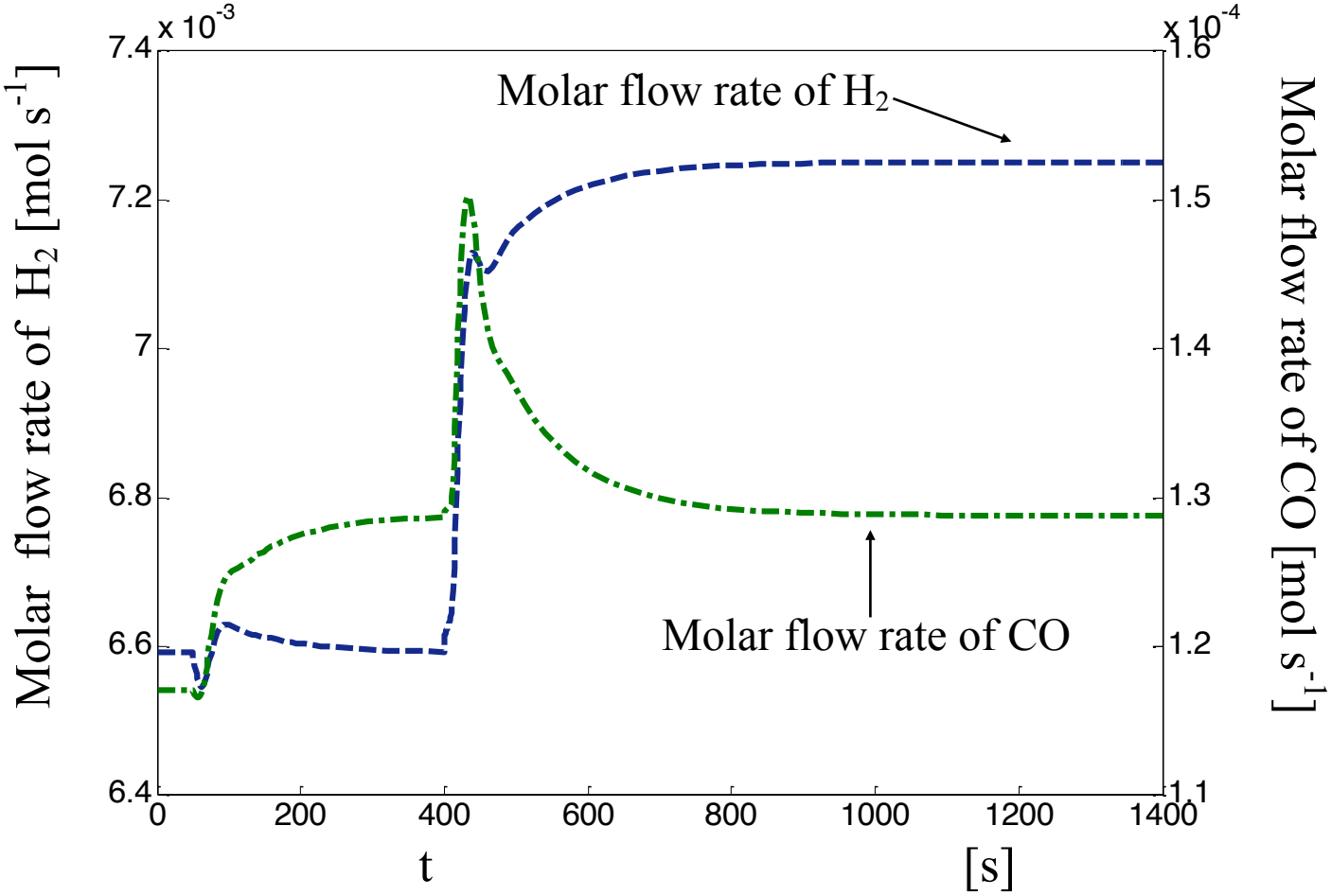
Table 1. Control structures

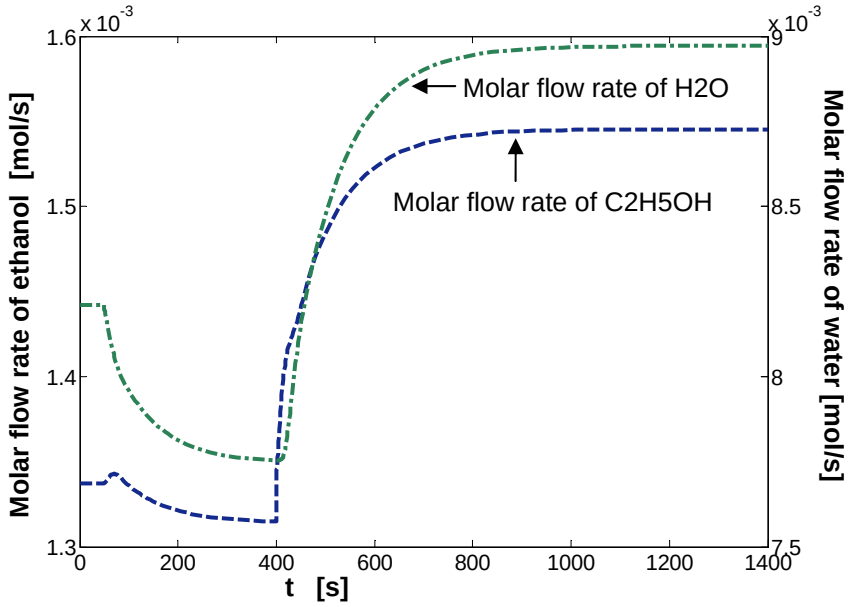
	$F_{C2H5OH,e}$ 10^{-3} [mol/s]	$F_{H2O,e}$ 10^{-3} [mol/s]	$T_{gas,e}$ [K]	$T_{F,S1}$ [K]	$T_{F,S2}$ [K]	$T_{F,S3}$ [K]	$F_{H2,s}$ [mol/s]	$F_{CO,s}$ [mol/s]
OP_n	1.34	8.21	648	648	678	613	6.39 10^{-3}	1.34 10^{-4}

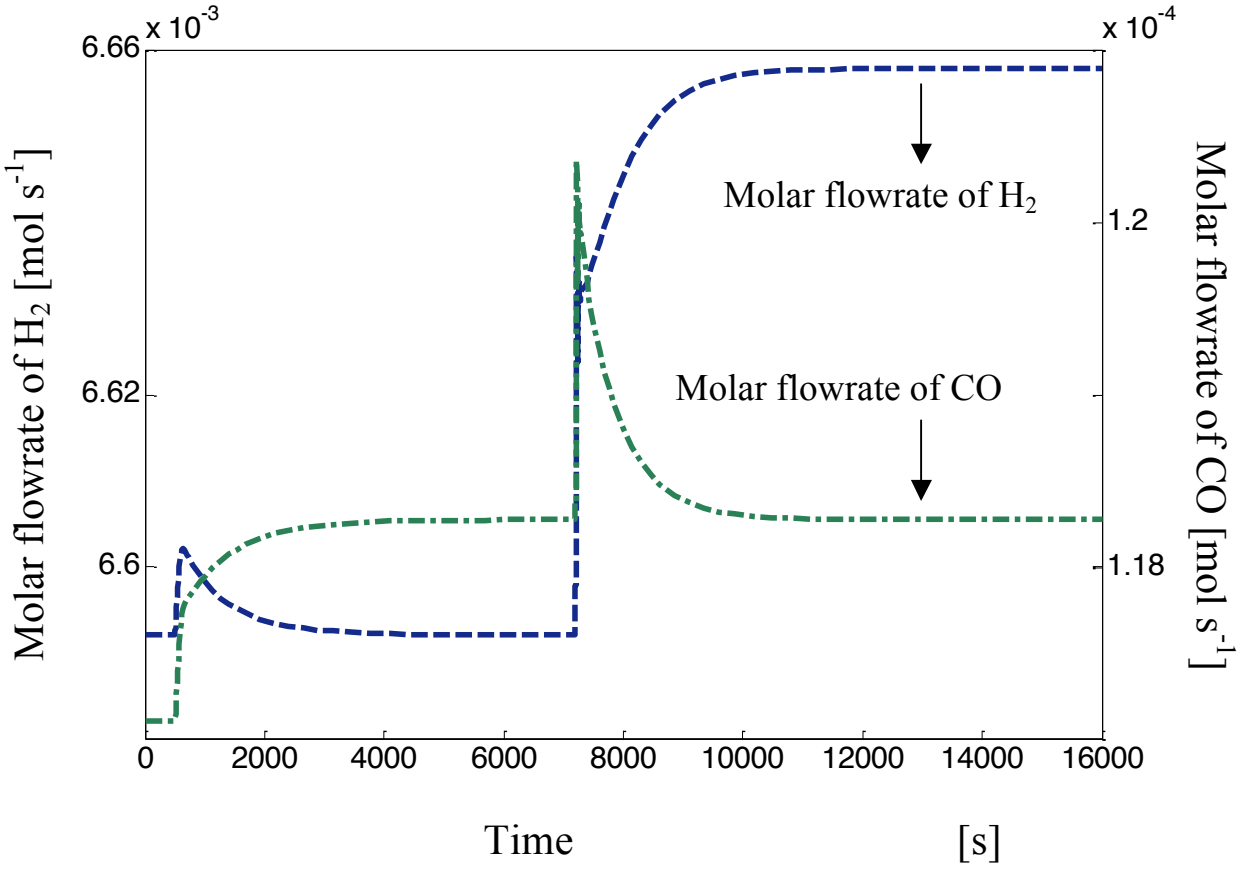
Table 2. Nominal operating conditions

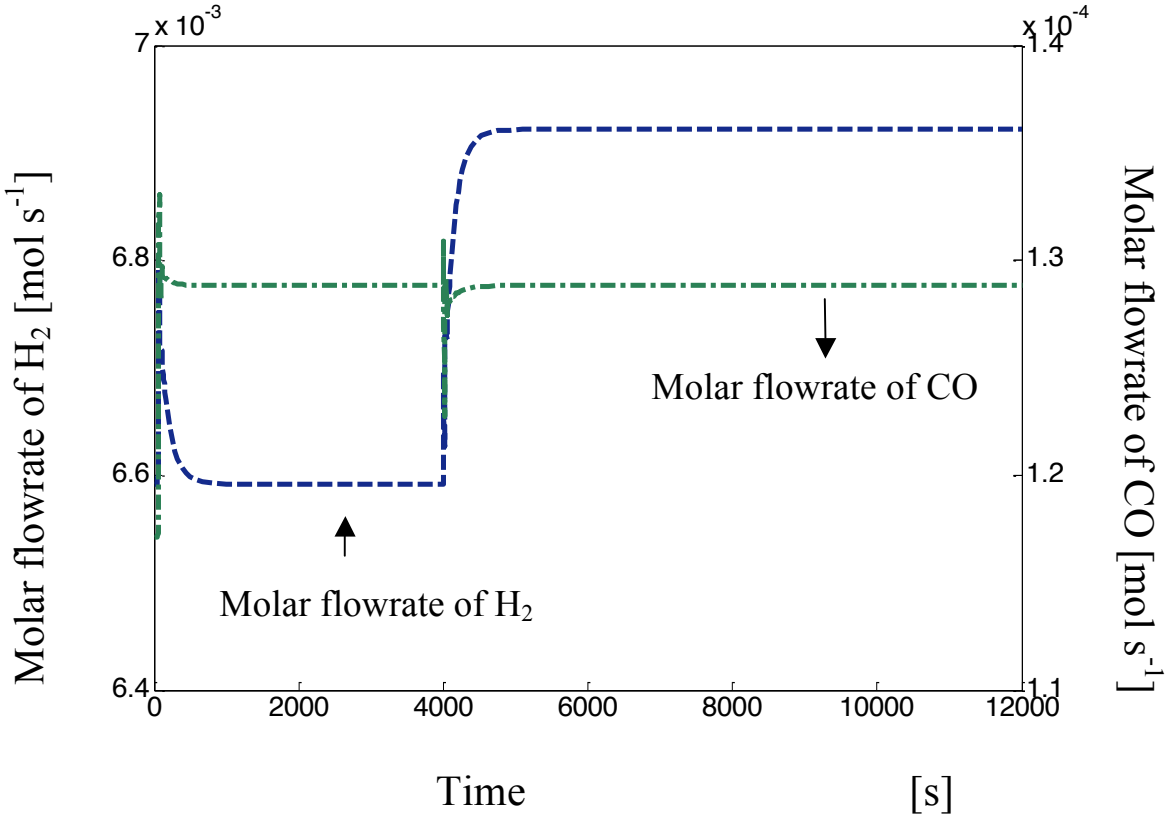
	Methods	Loop 1		Loop 2	
		Kp	Ki	Kp	Ki
Structure 1	T-E	$4x10^{-2}$	$7.3x10^{-3}$	$-9x10^{-1}$	$-6x10^{-1}$
Structure 2	Z-N	0.1	$4.3x10^{-3}$	$3.1x10^{5}$	$1.0x10^{4}$
Structure 3	T-E	0.6	$2.1x10^{-2}$	$2.8x10^{6}$	$9.3x10^{4}$
Structure 4	T-E	$9.9x10^{2}$	$2.1x10^{3}$	$2.8x10^{3}$	$5x10^{3}$
Structure 5	Z-N	$7.2x10^{4}$	$6.0x10^{2}$	$6.5x10^{5}$	$5.4x10^{5}$

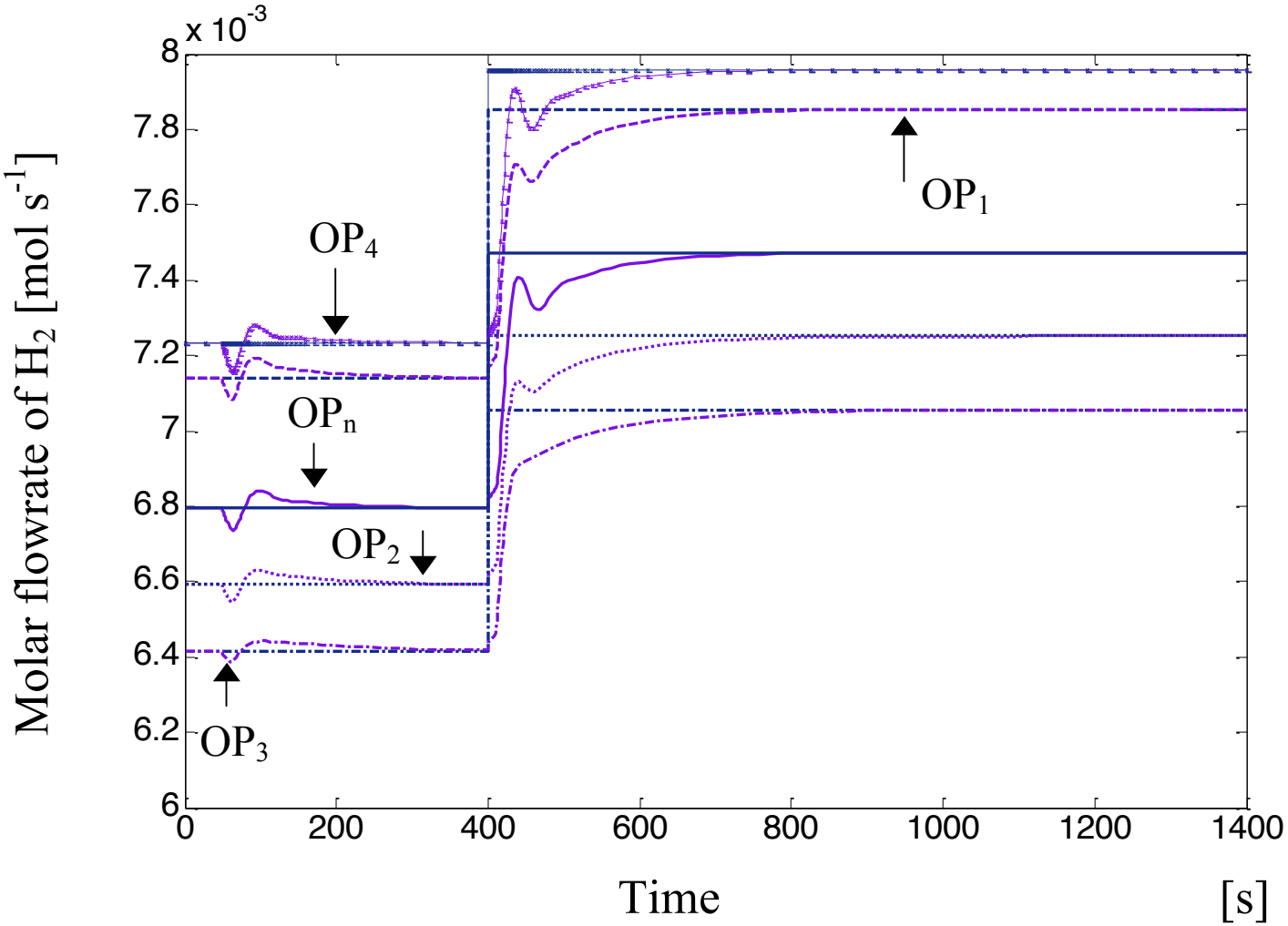
Table 3. PI parameters obtained by the Z-N and T-E methods

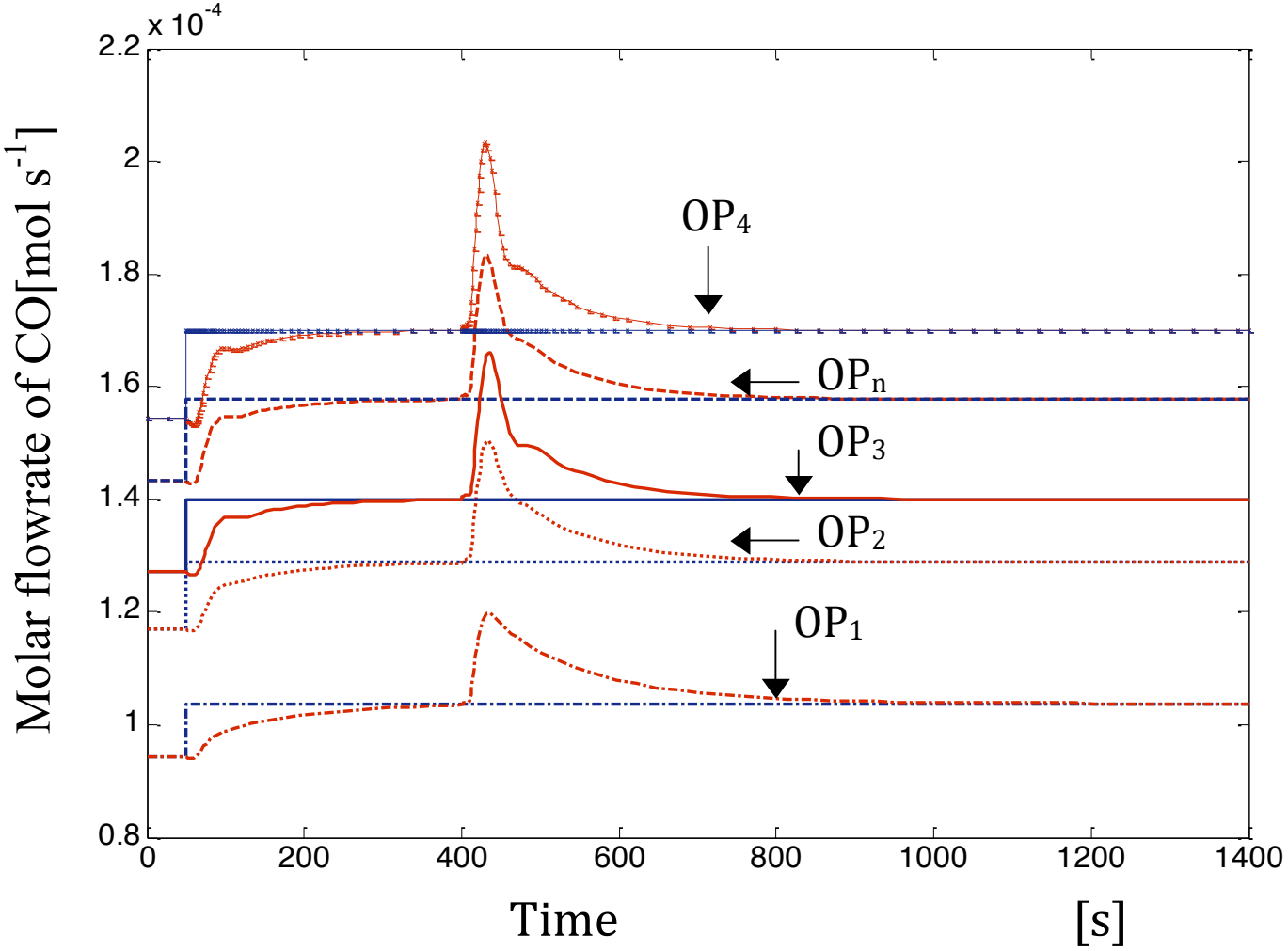

x 10^-3
x 10^-4
Molar flow rate of H2
Molar flow rate of CO
Molar flow rate of H2 [mol s-1]
Molar flow rate of CO [mol s-1]
7.4
7.2
7
6.8
6.6
6.4
1.6
1.5
1.4
1.3
1.2
1.1
0
200
400
600
800
1000
1200
1400
t
[s]


x 10^-3
1.6
1.5
1.4
1.3
Molar flow rate of ethanol [mol/s]
x 10^-3
9
8.5
8
7.5
Molar flow rate of water [mol/s]
Molar flow rate of H2O
Molar flow rate of C2H5OH
0
200
400
600
800
1000
1200
1400
t [s]


x 10^-3
6.66
6.62
6.6
x 10^-4
1.2
1.18
Molar flowrate of H2 [mol s-1]
Molar flowrate of CO [mol s-1]
Molar flowrate of H2
Molar flowrate of CO
0
2000
4000
6000
8000
10000
12000
14000
16000
Time
[s]


x 10^-3
x 10^-4
7
6.8
6.6
6.4
1.4
1.3
1.2
1.1
0
2000
4000
6000
8000
10000
12000
Molar flowrate of H2 [mol s-1]
Molar flowrate of CO [mol s-1]
Molar flowrate of CO
Molar flowrate of H2
Time
[s]


x 10^-3
8
7.8
7.6
7.4
7.2
7
6.8
6.6
6.4
6.2
6
0
200
400
600
800
1000
1200
1400
Molar flowrate of H2 [mol s-1]
Time
[s]
OP1
OP2
OP3
OP4
OPn


x 10^-4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0
200
400
600
800
1000
1200
1400
Molar flowrate of CO[mol s^-1]
Time
[s]
OP4
OPn
OP3
OP2
OP1