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Controllability Studies of Chemical Processes Based on the Concept of Passivity

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ASTRACT

This article presents an approach on controllability of nonlinear chemical processes based on passivity. The proposed method extents on the concept of Maya-Yescas and Aguilar (2003). The method divides the model system into controllable and uncontrollable parts. A controller can be designed by setting the controllable part equal to zero, so-called the perfect controller. For uncontrollable part, the storage and the supply rate functions are defined by implementing the same perfect controller to analyze the stability. If the uncontrollable part has the Kalman-Yacubovich-Popov (KYP) property, it is guaranteed to be stable and, therefore, the overall system would be controllable. The applications of proposed method are illustrated with two examples: 1) the four available control structures of heat exchanger network for one hot stream and two cold streams; and 2) the two process variables of continuous fermentation. The simulation results imply that the stability and the steady state of uncontrollable part can be considered only as the Lie derivative of a storage function. This technique can be extended to other nonlinear chemical processes as a tool for selecting the best input-output pairing to design the control structure.

Key words: controllability, passivity, nonlinear process, Kalman-Yacubovich-Popov (KYP) property, guaranteed stability

INTRODUCTION

General design of chemical processes has three decision steps: 1) structure of plant; 2) operational parameters, and 3) control structure. Consequently, evaluation is used to assess the performance of the processes by using controllability analysis. The control structure plays a major role on the controllability of processes (Lenhoff and Morari, 1982). Therefore, the control structure selection is an important factor in design and evaluation of chemical processes.

Several methods have been established to facilitate the selection of control structures. These are singular value, relative gain array (Bristol, 1966), condition number (Nguyen *et al*., 1988), disturbance cost (Lewin, 1996), passivity index (Bao *et al*., 2002), and others. These methods, developed for linear systems, have been extended to nonlinear system. For example, Cao *et al*. (1996) used a modified singular value and optimization technique to assess input-output controllability. Solovyev and Lewin (2003) extended the disturbance cost resiliency index to nonlinear systems.

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Recently, Maya-Yescas and Aguilar (2003) proposed an assessment technique for nonlinear systems based on the Lyapunov stability. The technique divides the system into two parts (controllable and uncontrollable) and proposes the input-output pairings at which uncontrollable parts are stable in the sense of Lyapunov stability.

Passivity index is a method for analysis of stability; it extended the concept of Lyapunov stability. A system is passive if it can be defined as a storage function (energy function like Lyapunov function) that is less than the supply function (Willems, 1972). Recently, Alonso and Ydstie (1996) and Ydstie and Alonso (1997) extended passivity concept to thermodynamics. The advantage of passivity approach is an easy definition of the storage and supply functions because these definitions are based on real energy such as the internal energy, entropy and exergy.

This article assesses a control structure based on the concept of passivity. The technique extends the work of Maya-Yescas and Aguilar (2003). The article develops a theory of passivity and proposed technique. The technique is tested with for heat exchanger networks (HENs) and a continuous fermentation process.

Theory

Consider the time invariant dynamical system:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{u}$$
$$\mathbf{y} = \mathbf{h}(\mathbf{x}) \qquad (1)$$

where $\mathbf{x} \in \mathbf{X} \subset \Re^n$, $\mathbf{u} \in \mathbf{U} \subset \Re^m$ and $\mathbf{y} \in \mathbf{Y} \subset \Re^n$ are state, control and output vectors, respectively, and **X**, **U** and **Y** are state, input and output spaces, respectively. The representation $\mathbf{x}(t) = j(t, t_0, \mathbf{x}_0, \mathbf{u})$ is used to denote the state at time t reached from the initial state $\mathbf{x}_0$ at t_0.

Definition 1 *Passive Systems* (Willems, 1972)

A system (Eq.1) is said to be passive if it is a dissipative system with supply rate $w(t) = \mathbf{y}^{\mathrm{T}}(t)\mathbf{u}(t)$ and the storage function satisfying $S(0) = 0$. That is,

$$S(\mathbf{x}) - S(\mathbf{x}_0) \le \int_0^t \mathbf{y}^{\mathrm{T}}(\tau)\mathbf{u}(\tau)d\tau \qquad (2)$$

Definition 2 *Kalman-Yacubovich-Popov (KYP) Property* (Hill and Moylan, 1976, 1977, 1980a, 1980b)

A system (Eq.1) has the KYP property if there exists a C^1 (continuous real number) nonnegative function S: $\mathbf{X} \rightarrow \Re$, with $S(0) = 0$, such that

$$L_{\mathrm{f}}S(\mathbf{x}) \le 0$$
$$L_{\mathrm{g}}S(\mathbf{x}) = \mathrm{h}(\mathbf{x}) \qquad (3)$$

for each $\mathbf{x} \in \mathbf{X}$.

Conversely, the passive system having C^1 storage function has KYP **properties** (Hill and Moylan, 1976).

To assess controllability, the system (Eq.1) is divided into two parts

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{u} \rightarrow \begin{cases} \dot{\mathbf{x}}_C = \mathbf{f}_C(\mathbf{x}) + \mathbf{g}_C(\mathbf{x})\mathbf{u} \\ \dot{\mathbf{x}}_D = \mathbf{f}_D(\mathbf{x}) + \mathbf{g}_D(\mathbf{x})\mathbf{u} \end{cases} \qquad (4)$$

where subscript C and D refers to controlled and uncontrolled parts, respectively. At the equilibrium point of controllable part, $\mathbf{x}_C$, **is made** equal to zero by using the input

$$\mathbf{u} = \mathbf{u}^{sp} = -\mathbf{g}_C^{-1}(\mathbf{x})\mathbf{f}_C(\mathbf{x}) \qquad (5)$$

Substituting **u** (Eq.5) into uncontrollable parts

$$\dot{\mathbf{x}}_D = \mathbf{f}_D(\mathbf{x}) - \mathbf{g}_D(\mathbf{x}) - \mathbf{g}_C^{-1}(\mathbf{x})\mathbf{f}_C(\mathbf{x}) \qquad (6)$$

Proposition 1

The system (Eq.1) will be stable for all $t > 0$, if and only if, $L_{\mathbf{f}_D} S \le 0$ and $L_{\mathbf{g}_D} S = \mathbf{h}(\mathbf{x}_D)$ i.e. if $\dot{\mathbf{x}}_D$ is a passive system.

Proof

Consider the uncontrolled part (Eq.6) and define the storage function, $S(\mathbf{x}_D)$. The system $\dot{\mathbf{x}}_D$ will be stable if the derivative of storage function is less than the supply rate function, $w = \mathbf{u}^{\mathbf{T}}\mathbf{y} = \mathbf{u}^{\mathbf{T}}\mathbf{h}(\mathbf{x})$

$$\dot{s}(\mathbf{x}_D) = \frac{\partial s(\mathbf{x}_D)}{\partial \mathbf{x}_D}\dot{x}_D = \frac{\partial s(\mathbf{x}_D)}{\partial \mathbf{x}_D}\left[\mathbf{f}_D(\mathbf{x}) + \mathbf{g}_D(\mathbf{x})\mathbf{u}^{sp}\right] \le \mathbf{x}^T\mathbf{h}(\mathbf{x}) \quad (7)$$

for $\mathbf{u} = \mathbf{u}^{sp}$ and by using the KYP property (see *Definition 2*), we obtain

$$L_{\mathbf{f}_D} S \le 0 \text{ , and} \quad (8)$$

$$L_{\mathbf{g}_D} S = \mathbf{h}(\mathbf{x}) \quad (9)$$

i.e. the uncontrolled part is a passive system that corresponds to the KYP property.

RESULTS AND DISCUSSION

Case study I: Heat Exchanger Network (HEN)

The HEN used here has three streams; one hot stream and two cold streams. The network process begins with the heat exchanger of the hot stream (H) with the cold stream one (C1) at the heat exchanger A. Then, the output hot stream is exchanged again with the cold stream two (C2) at the heat exchanger B. In order to analyze controllability and minimize the energy utility, the dynamic aspect must be determined by selecting the positions to install valves and heat utilities. The four control structures of the HEN are shown in Figures 1 and their parameters are given in Table 1. Before modeling the HEN, the following assumptions are made for all structures:

1. Heat capacity is constant because of narrow range temperature difference.
2. Transportation lag in the pipe is zero.
3. There is no heat loss in the pipe due to perfect insulation.

The general dynamic model of HENs are defined as

$$\frac{dE_{h,i}}{dt} = \left(FC_P\right)_{h,i}^{in} T_{h,i}^{in} - \left(FC_P\right)_{h,i}^{out} T_{h,i}^{out} - \sum (UA)_k \Delta T_{LN,k} - Q_{c,i} \quad (10)$$

$$\frac{dE_{c,j}}{dt} = \left(FC_P\right)_{c,j}^{in} T_{c,j}^{in} - \left(FC_P\right)_{c,j}^{out} T_{c,j}^{out} - \sum (UA)_k \Delta T_{LN,k} - Q_{h,j} \quad (11)$$

where

$$\Delta T_{LN} = \frac{\left(T_{h,i}^{in*} - T_{c,j}^{out*}\right) - \left(T_{h,i}^{out*} - T_{c,j}^{in*}\right)}{\ln \dfrac{\left(T_{h,i}^{in*} - T_{c,j}^{out*}\right)}{\left(T_{h,i}^{out*} - T_{c,j}^{in*}\right)}} \quad (12)$$

$$T_{h,i}^{mix} = u_k T_{h,i}^{in*} + (1 - u_k) T_{h,i}^{out*} \quad (13)$$

$$T_{c,j}^{mix} = u_k T_{c,j}^{in*} + (1 - u_k) T_{c,j}^{out*} \quad (14)$$

$$Q_{c,i} = \left(FC_P\right)_{h,i}\left(T_{h,i}^{out*} - T_{h,i}^{target}\right) \quad (15)$$

$$Q_{h,j} = \left(FC_P\right)_{c,j}\left(T_{c,j}^{target} - T_{c,j}^{out*}\right) \quad (16)$$

The storage functions for all streams in the entropy form can be defined (Coffey *et al*., 2000) as follows:

$$S(E) = \left(\frac{1}{T^{target}}\right)\left(E - E^{target}\right) + \left(\bar{A}^* - \bar{A}\right), \quad S(0) \ge 0 \quad (17)$$

$$\frac{dS(E)}{dt} = \frac{dS(E)}{dE}\frac{dE}{dt} = -\left(\frac{1}{T^{out}} - \frac{1}{T^{target}}\right)^T \frac{dE}{dt} \quad (18)$$

where $\bar{A}$ is the total exergy and superscript $\bar{A}^*$ denotes the reference state.

The uncontrollable part will be stable if the derivative of storage function (Eq.18) is less than supply rate, i.e.

$$\dot{S}(E) = -\left(\frac{1}{T^{out}} - \frac{1}{T^{target}}\right)\frac{dE}{dt} \le w \quad (19)$$

where w is the supply rate ($u^T y$). Note that the manuplated variable, u, does not exist in the uncontrollable part. In order to satisfy the

Table 1 Parameters for heat exchanger network.

Stream No.	C_P (kW/°C)	T^{in} (°C)	T^{target} (°C)
H	1.0	190 ± 10	30
C1	1.5	80	160
C2	0.5	20	130

Note: Overall heat transfer coefficient UA_A = 0.523 kW/°C and UA_B = 1.322 kW/°C.
Source: Glemmestad *et al*. (1999)

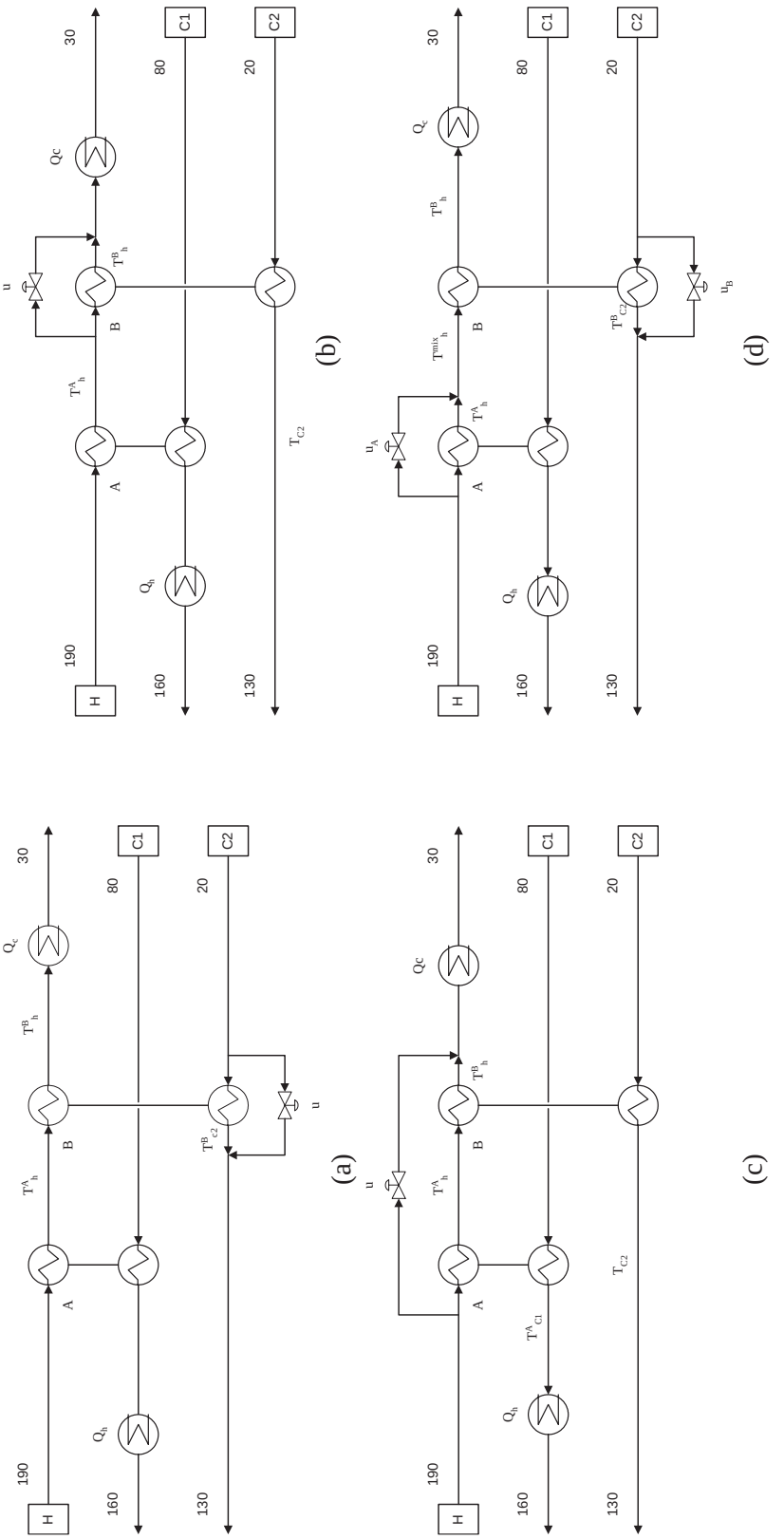


Figure 1 Heat exchanger network: (a) type I, (b) type II, (c) type III, (d) type IV.

Proposition 1, Eq.(19) must be less than zero. The input and output temperatures for open-loop (no bypass) are shown in Figure 2(a) and (b), respectively. The output temperature responses of each stream for all structures are shown in Figure 3. Figure 4 represents the controller's action on the target streams for each structure.

Concerning the HEN structure I, Figure 2(a) shows that stream C2 is not completely controllable. Because, initially, all streams remain at the set point when the stream H was stepped to 200 °C, the stream can largely exchange energy at

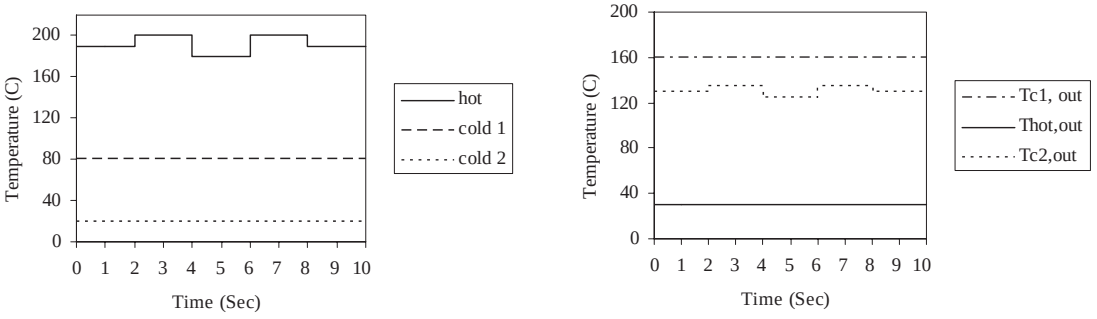


Figure 2 (a) Input temperature for each streams, (b) output temperature when no bypass.

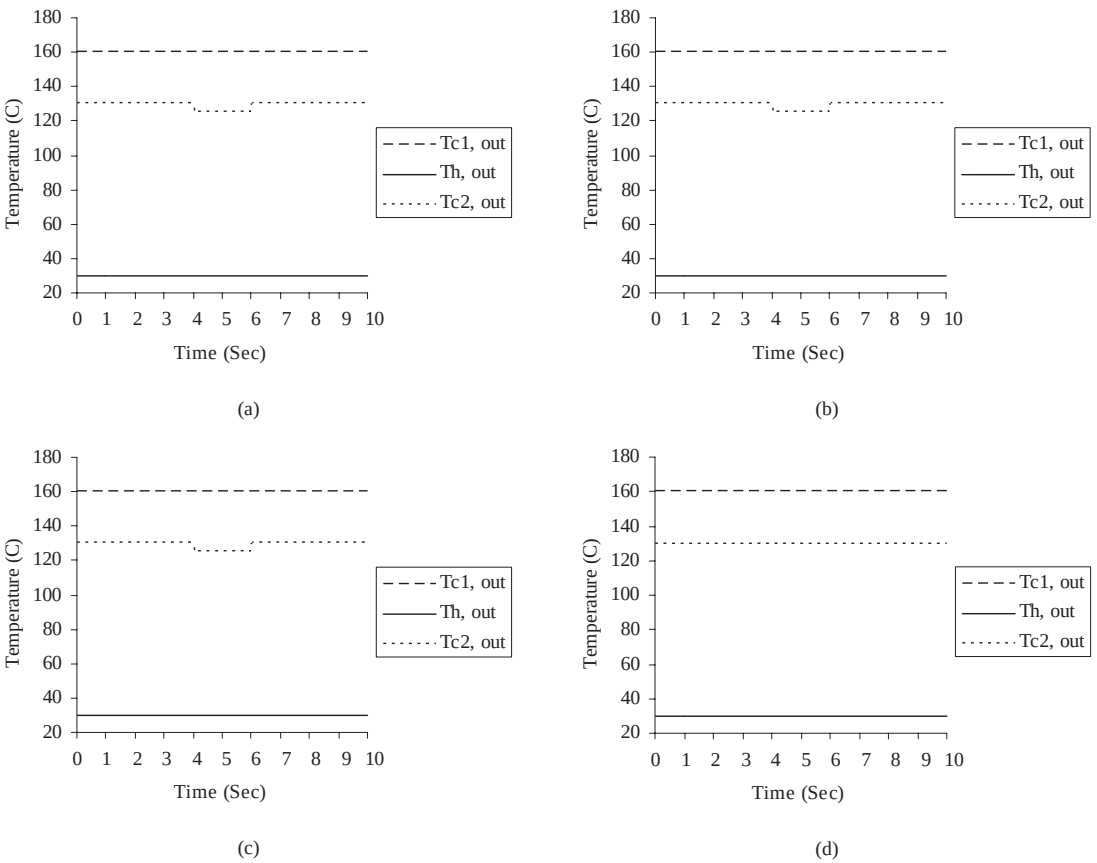


Figure 3 Output temperature response (a) structure I, (b) structure II, (c) structure III, (d) structure IV.

the heat exchanger A. This means that stream C1 can receive large amount of energy and thus reduces the utilities consumptions. After being exchanged at cell A, the stream H can be further exchanged at cell B. This requires the valve (u) to be opened (7.5%) to maintain the temperature of stream C2. However, the stream H must consume more utilities to maintain the temperature target.

After 2 seconds, the input temperature of stream H reduces to 180 °C. This affects stream C1 because the energy is exchanged less, so it consumes more utilities. For the stream C2, the energy is exchanged less. Therefore, the valve must be completely closed to increase the exchanged energy. However, the amount of exchanged energy is not enough to increase the temperature of stream C2. At the 6th second, the input temperature of stream H increases to 200 °C again and the behavior of the streams, valve, and utility consumption are the same as explained above.

To consider the stability of uncontrollable part, the utility consumption can be considered because it directly affects the output temperature. If the utilities can raise the output temperature to the target temperature, it will satisfy Eq. (19). This means that if the behavior of the utilities is stable, the uncontrollable parts will be stable.

Considering the HEN structure II, the behaviors of all variables are the same as structure I because all parameters and structure are the same as structure I except the position of valve. However, if valve of structure II is opened to 26.0 %, it is more than structure I. Depending on heat capity flow rate (FC_p), The value on steam H should be opened higher than it was in structure I to transfer the some amout of heat.

Comparing these two structures, structure I is preferred because valve behavior directly affects the process variable (stream C2) that satisfies the heuristics, and the percent of valve opening is less than in structure II. These differences affect the cost and the size of valve.

Considering the HEN structure III, the responses of all temperatures are shown in Figure 3(c). The stream C2 is not be completely controllable; the reason is the same as for structures I and II. However, the overall plant is stable because the behaviors of utilities are stable. The valve is 16.0 % open to reject the disturbance from the stream H when input temperature is stepped up to 200 °C and completely closed when input temperature is reduced to 180 °C.

From the above three cases, the main problem is that when the temperature of stream H reduces to 180°C the exchanged energy is not enough to increase the temperature of stream C2. This problem can be overcome by dividing the energy before being exchanged at heat exchanger A to heat exchanger B by installing valve u_A at exchanger A to divide the energy and valve u_B at the heat exchanger B to control the stream C2. This can be seen in structure IV.

Figure 3(d) shows that all the output temperatures are controllable. When the temperature of stream H steps to 200 °C, the valve u_B is open 7.5 % to reject the disturbance and valve u_A is completely closed. The behavior is the same as in structure I. At the 4th second, the temperature of stream H reduces to 180 °C, even though valve u_B is completely closed the temperature of stream C2 cannot be increased to target. Since the valve u_A must be opened 50 % (see Figure 4(d)) to divide the energy before going into heat exchanger A. This affects stream C1 and it must consume more utilities. At the 6th second, the temperature of stream H increases to 200 °C again and both valves turn to the same position as at the 2nd second. The utility consumption of the structure IV is 1.48 MJ per 10 second. The overall plant is stable because the behavior of utilities is stable. Table 2 compares the utility consumption for all structures. The table shows that structure IV consumes the most utility. However structure IV is preferred because it can keep all output streams at the target temperature.

Case study II: Continuous Fermentation

Continuous fermentations have strongly nonlinear characteristics and their operation is known to be difficult to reproduce and control. The fermentation operation can be represented by the growth rate model with the following assumption:

1. Perfectly stirred lumped system.
2. Isothermal operation.
3. Constant physico-chemical properties.

Model of the continuous fermentation

$$\frac{dX}{dt} = \mu(S_s)X - X\frac{F}{V} \tag{20}$$

$$\frac{dS_S}{dt} = \left(-\frac{\mu(S_S)}{Y} - m\right)X - \left(S_s - S_f\right)\frac{F}{V} \tag{21}$$

where

$$\mu(S_s) = \mu_{\max}\frac{S_s}{K_2 S_s^2 + S_s + K_1} \tag{22}$$

This case study is divided into two subcases. One involves the pairing of biomass concentration and flow rate. The second subcase pairs the substrate and flow rate.

Subcase I: Controllable part is X and uncontrollable part is S_S. The storage function for uncontrollable part can be defined as follows:

$$S(S_s) = \frac{1}{2K_c}S_s^2, \quad S(0) = 0 \tag{23}$$

where $K_c = -(S_s^* - S_f)$ and supply function is defined as

$$w = \frac{F}{V}S_s \tag{24}$$

Therefore, the passivity equation for uncontrolled part can be written as

Table 2 Comparison of heat utility consumption for all structures.

Structure	Utility consumption (J) per 10 second
No bypass	1450092
I	1460896
II	1460896
III	1469183
IV*	1480936

Table 3 Parameters for the continuous fermentation.

Parameters	Meaning	Value
μ_{max}	Maximum specific growth rate	1 dm^3/h
K_1	Saturation parameter	0.03 g/dm^3
K_2	Inhibition parameter	0.5 dm^3/g
m	Maintenance coefficient	0.01 h^{-1}
V	Volume of fermentor	4 dm^3
S_f	Substrate feed concentration	10 g/dm^3
Y	Yield coefficient	0.4 g/g
F^*	Steady state flow rate	3.2089 dm^3/h
S_s^*	Steady state substrate concentration	0.2187 g/dm^3
X^*	Steady state biomass concentration	0.48907 g/dm^3

Source: Szederkâyi *et al*. (2002) and Kuhlmann and Bogle (2001)

$$\frac{dS(S_s)}{dt} = \frac{dS(S_s)}{dS_s}\frac{dS_s}{dt} = K_c^{-1}S_s\frac{dS_s}{dt} \le \frac{F}{C}S_s \quad (25)$$

$$K_c^{-1}S_s\frac{dS_s}{dt} = K_c^{-1}S_s\left[\left(-\frac{\mu(S_s)}{Y}-m\right)X-\left(S_s-S_f\right)\frac{F}{V}\right] \le \frac{F}{V}S_s \quad (26)$$

Applying the KYP lemma, we obtain

$$L_fS(S_s) = K_c^{-1}S_s\left(-\frac{\mu(S_s)}{Y}-m\right)X \le 0\text{, and} \quad (27)$$

$$L_gS(S_s) = -\left(S_s-S_f\right)K_c^{-1}S_s = S_s \quad (28)$$

Substituting $K_c = -(S_s^* - S_f)$ into Eqs.(27) and (28) gives the result corresponding to the *Proposition 1*. The response of two outputs (*X*, S_S) and input (*F*/*V*) are shown in the Figures 4 and 5, respectively.

For the first subcase, Figure 4 shows that the response of *X* always stays at the equilibrium point (4.8907 g/dm^3) even as S_S increases from 0.2187 g/dm^3 to 7.9579 g/dm^3 and *F* decreases from 3.2089 dm^3/h to 0.80276 dm^3/h (Figure 5). This means that the biomass concentration is stable although the disturbance, S_S, increases. The manipulated variable, *F*, is decreased to adjust the concentration of *X* in the fermentor due to increasing of S_S.

Subcase II: Controllable part is S_S and uncontrollable part is *X*. The storage function for uncontrollable part is defined as follows:

$$S(X) = \frac{1}{2K_c}X^{-2},\ \ S(0) = 0 \quad (29)$$

where and supply function is defined as

$$w = \frac{F}{V}X \quad (30)$$

The passivity equation for uncontrolled part can be written as

$$\frac{dS(X)}{dt} = \frac{dS(X)}{dX}\frac{dX}{dt} = K_c^{-1}X\frac{dX}{dt} \le \frac{F}{V}X \quad (31)$$

$$K_c^{-1}X\frac{dX}{dt} = K_c^{-1}X\left[\mu(S_s)X - X\frac{F}{V}\right] \le \frac{F}{V}X \quad (32)$$

Applying the KYP lemma gives

$$L_fS(X) = K_c^{-1}X\mu(S_s)X \le 0\text{, and} \quad (33)$$

$$L_gS(X) = \frac{X^2}{X^*} = X \quad (34)$$

The response of two outputs (*X*, S_S) and input (*F*/*V*) are shown in the Figures 7 and 8, respectively. The L_fS and L_gS values are illustrated over 30 second.

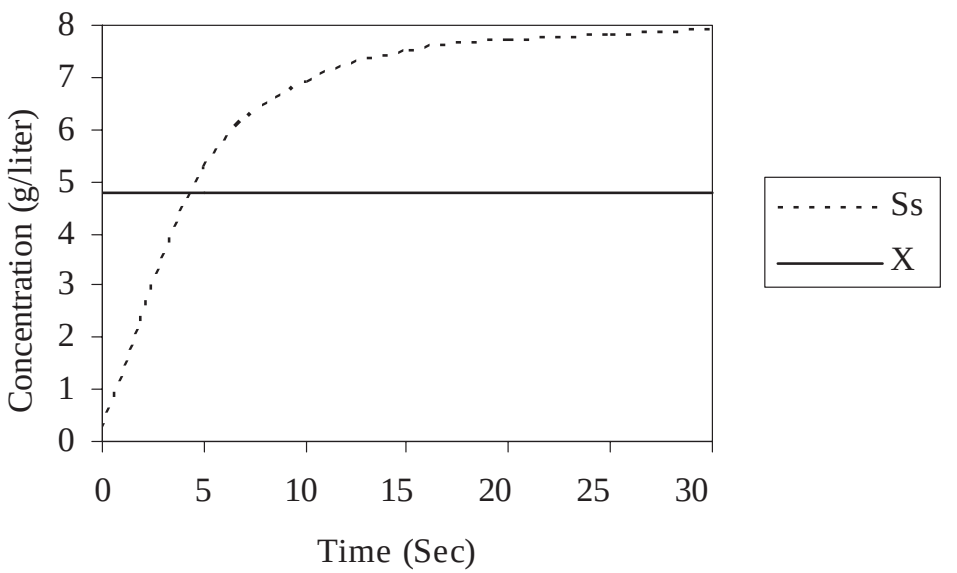


Figure 4 Response of biomass and substrate when biomass is the controllable part.

Considering the second subcase, Figure 6 shows that the controllable part, S_S, does not go to steady state; instead it reaches 0.5000 g/dm^3. However, F is decreased to attempt to reduce the S_S, but F is limited to nearly zero. If flow rate is zero or negative, it means that, in practice, F does not feed input but it sucks the substrate and biomass from the fermentor (see Figure 7).

CONCLUSION

Passivity is the method of analyzing the stability of nonlinear chemical processes. The concept of passivity is extended from the Lyapunov stability. However, the Lyapunov stability is difficult to implement because it requires a proper choice of Lyapunov functions.

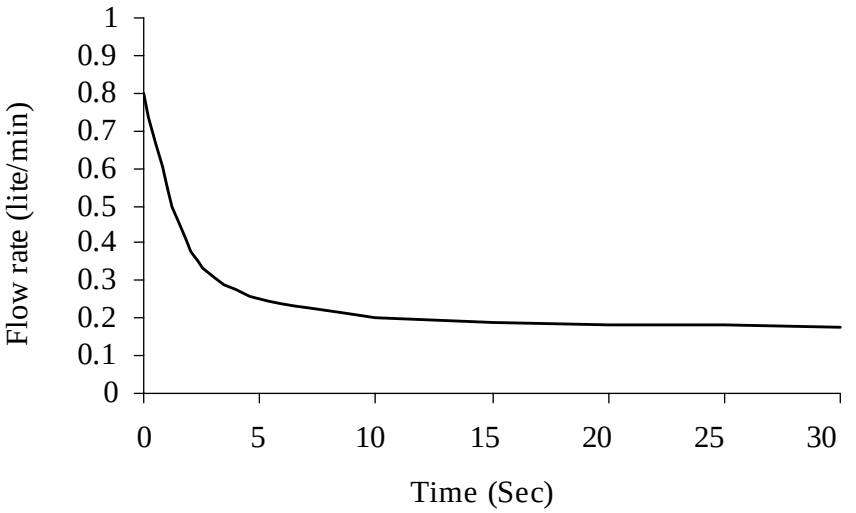


Figure 5 Response of feed flow rate when biomass is the controllable part.

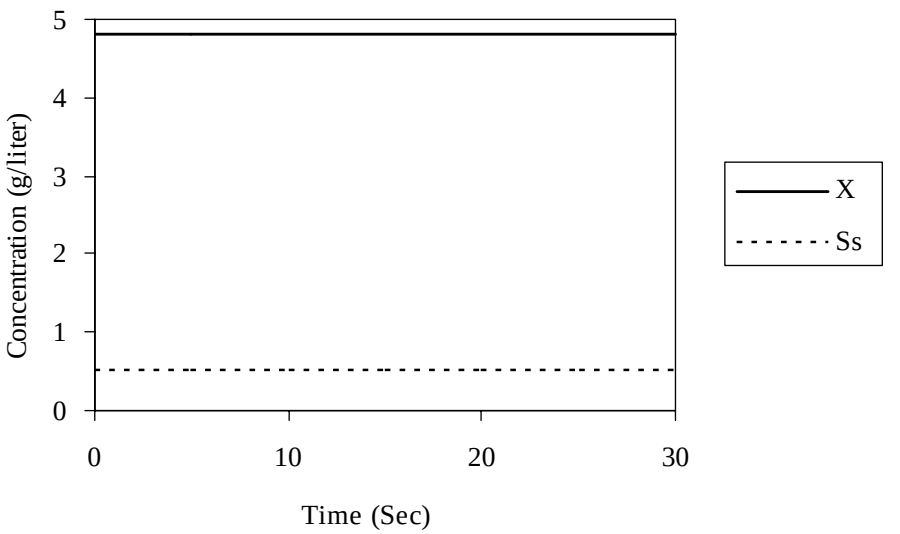


Figure 6 Response of biomass and substrate when substrate is the controllable part.

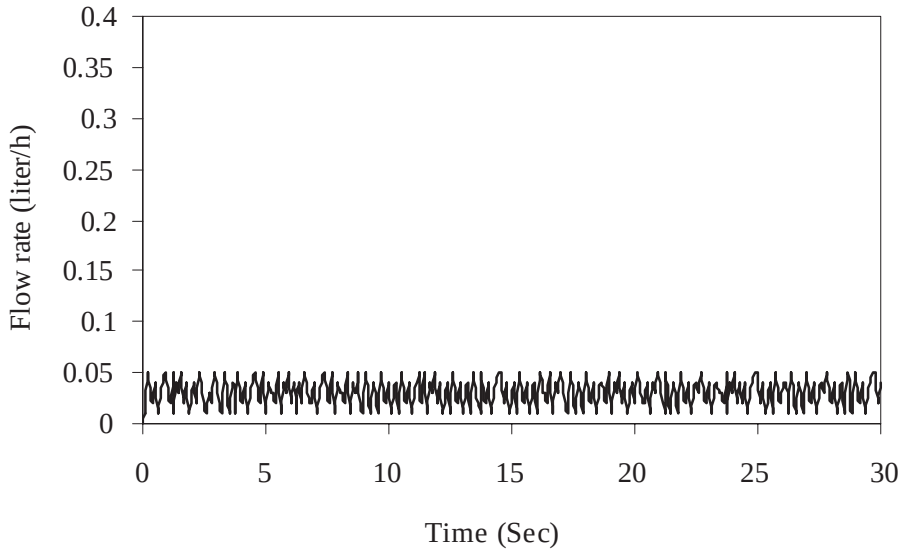


Figure 7 Response of feed flow rate when substrate is the controllable part

The passivity-based thermodynamics proposed by Alonso and Ydstie (1996) is a useful method for choosing the storage function (or Lyapunov function) because it is very close to the physical energy such as the internal energy, entropy, or exergy. The passivity method enables an easy analysis of the stability of nonlinear chemical processes.

Controllability-based passivity technique proposed in this article is a new approach to assess controllability. The procedure starts by dividing the system into controllable and uncontrollable parts and defining the storage function for uncontrollable part in order to make it stable. This concept is implemented for a heat exchanger network and continuous fermentation. The example of heat exchanger network has one hot stream and two cold streams. The four control structure configurations of the heat exchanger were studied and the technique proposed was used to decide which structure was the most suitable. The results show that the structure IV is preferred because it enables the process variable to go to the set point even though it consumes the maximum utility. For the continuous fermentation, two choices of process variables (biomass and substrate), but only one manipulated variable, flow rate, are compared. The result shows that the pairing of biomass-flow rate is preferred because it gives L_fS of uncontrollable part to be less than zero; consequently, the uncontrollable part is guaranteed to be stable. Moreover, L_gS of a system can be used as a criterion to choose the process variable.

This concept can be used as a tool to screen out the unsuitable process variables. However, this technique is only applicable for models defined in the state space. Further work is required to cover the systems defined in input-output space. Furthermore, the robustness of this approach still needs to be addressed with some more examples.

ACKNOWLEDGEMENT

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Nomenclatures

Greek Letters

φ	State transition
μ	Growth rate
τ	Time constant
$\Re$	Set of real number

SYMBOLS

$\overline{A}$	Helmotz energy (J)
Cp	Heat capacity (kW/C)
E	Stream energy (J)
F	Flow rate
f	Matrix function
g	Matrix function
h	Matrix function
L_fS	Lie derivative of S defined as $L_f S = \frac{\partial S(x)}{\partial x} f(x)$
L_gS	Lie derivative of S defined as $L_g S = \frac{\partial S(x)}{\partial x} g(x)$
Q	Heat utility
S	Storage function
T	Temperature
t	time
U	Set of input vector
u	Input vector
u	Manipulated variable (bypass)
V	Volume
w	Supply rate function
X	Set of state variables
X	Biomass concentration
x	State variable
Y	Set of out put variable
y	Output variable

SUPERSCRIPTS

*	Steady state
	Derivative respect to time

SUBSCRIPTS

c	Cold
f	Substrate feed concentration
h	hot
0, 1	Number of state

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