Literature Review on Nonnegative Dynamics, Compartmental Modeling and Vector Dissipativity Theory

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Abstract

Nonnegative dynamical system models are derived from mass and energy balance considerations that involves dynamic states whose values are nonnegative. These model are widespread in biological and ecological sciences and play a key role in the understanding of these processes.An unified framework(linear & nonlinear) involving compartmetal modeling, stability analysis and vector dissipativity theory was developed in [1, 2, 3, 4]. This work contains systematic review on these subjects and some rough ideas about their applications in chemical process control.

Contents

1 Introduction

Chemical process dynamics involves mass recycle and heat intergration. Traditionally, the model is based on state space with interaction as the direct connection bewteen inputs and outputs of subsystem. This will lead to a complex generalized state space model whose phyical meaning is lost. When the system grows into plantwide complexity, it is not adequately to capture the real interconnection.

The compartmental model is a natural way to describe energy flow model involving heat flow, mass flow, work energy, and chemical reactions. A state-space dynamical system model that captures the key aspercts of thermodynamics, including its fundamental laws. So maybe, the compartmental modeling would be an alternative solution to the plantwide complexity of chemical process. And some control stragies combining dissipativity and MPC can be developed and form a distributed control framework.

2 Nonnegative Dynamics

2.1 Mathematical Preliminaries

Defination 2.1. Let $A \in \mathbb{R}^{m\times n}$. Then A is **nonnegative** (resp., **positive**) if $A_{ij} \geqslant 0$ (resp., $A_{ij} > 0$) for all $i = 1, \cdots, m$ and $j = 1, \cdots, n$.

Defination 2.2. Let $T > 0$. A real function $u : [0, T] \to \mathbb{R}^m$ is a nonegative (resp., positive) function if $u(t) \geqslant\geqslant 0$ (resp., $u(t) \gg 0$), which means $u_i(t) \geqslant 0$ (resp., $u_i(t) > 0$) for $i = 1, \cdots, m$.

Defination 2.3. Let $A \in \mathbb{R}^{n\times n}$. A is a **Z-matrix** if $A_{ij} \leqslant 0, i, j = 1, \cdots, n, i \neq j$. A is an **M-matrix** (resp., nonsingular M-matrix) if A is a Z-matrix and all the principal minors of A are nonnegative (resp., positive). A is **essentially nonnegative** if -A is a Z-matrix, which means $A_{ij} \geqslant 0, \forall i, j = 1, \cdots, n, i \neq j$.

Lemma 2.1. *Assume A is a Z-matrix. Then the following statement are equivalent:*

(i) *A is an M-matrix.*

(ii) $\exists \alpha > 0, B \geqslant\geqslant 0$ *s.t.* $\alpha > \rho(B)$ *and* $A = \alpha I - B$.

(iii) *Re*$\lambda \geq 0$, $\lambda \in \operatorname{spec}(A)$.

(iv) *If* $\lambda \in \operatorname{spec}(A)$, *then either* $\lambda = 0$ *or* $\lambda > 0$.

Furthermore, in the case where A is a nonsigular Z-matrix, then the following statements are equivlent:

(v) *A is a nonsingular M-matrix.*

(vi) *det*$(A) \neq 0$ *and* $A^{-1} \geqslant\geqslant 0$.

(vii) $y \in \mathbb{R}^n, y \geqslant\geqslant 0$, *then* $\exists x \in \mathbb{R}^n, x \geqslant\geqslant 0$ *s.t.* $Ax = y$.

(viii) $\exists x \in \mathbb{R}^n, x \geqslant\geqslant 0$, *s.t.* $Ax \gg 0$.

(ix) $\exists x \in \mathbb{R}^n, x \gg 0$, *s.t.* $Ax \gg 0$.

2.2 Stability of linear case

Consider the linear dynamical system of the form

$$\dot{x} = Ax, \qquad x(0) = x_0, t \geqslant 0 \tag{1}$$

Lemma 2.2. *Let* $A \in \mathbb{R}^{n\times n}$. *A is essentially nonegative iff* e^{At} *is nonnegative for all* $t \geqslant 0$. *Furthermore, if A is essentially nonnegative and* $x_0 \geqslant\geqslant 0$, *then* $x(t) \geqslant\geqslant 0$ *and Sys.1 is called* ***linear nonnegative dynamical system****.*

Defination 2.4. The quilibrium solution $x(t) = x_e$ of Sys.1 is

- **Lyapunov stable** if, $\forall \epsilon > 0, \exists \delta = \delta(\epsilon) > 0$ s.t. if $x_0 \in \mathcal{B}_\delta(x_e) \cap \overline{\mathbb{R}}_+^n$, then $x(t) \in \mathcal{B}_\delta(x_e) \cap \overline{\mathbb{R}}_+^n, t \geqslant 0$.
- **semistable** if it is Lyapunove stable and $\exists \delta > 0$ s.t. if $x_0 \in \mathcal{B}_\delta(x_e) \cap \overline{\mathbb{R}}_+^n$, then $\lim_{t\to\infty} x(t)$ exists and converges to a Lyapunov stable equilibrium point.
- **asymptotically stable** if it is Lyapunov stable and $\exists \delta > 0$ s.t. if $x_0 \in \mathcal{B}_\delta(x_e) \cap \overline{\mathbb{R}}_+^n$, then $\lim_{t\to\infty} x(t) = x_e$.
- **globally asmptotically stable** if it is asymptotically stable respect to all $x_0 \in \mathbb{R}^n$.

Theorem 2.1. *Let* $A \in \mathbb{R}^{n\times n}$ *be essentially nonnegative. If* $\exists p, r \in \mathbb{R}^n$ *s.t.* $p \gg 0, r \geqslant\geqslant 0$ *statisfy*

$$0 = A^T p + r \tag{2}$$

then the following properties hold:

(i) *-A is an M-matrix.*

(ii) *If* $\lambda \in \operatorname{spec}(A)$, *then either* $\lambda = 0$ *or* $\lambda > 0$.

(iii) *ind*$(A) \leqslant 1$, *so A has generalized group inverse* $A^\#$.

(iv) *A is semistable and* $\lim_{t\to\infty} e^{At} = I - AA^\# \geqslant\geqslant 0$.

(v) $\mathcal{R}(A) = \mathcal{N}(I - AA^\#)$, $\mathcal{N}(A) = \mathcal{R}(I - AA^\#)$.

(vi) $\int_0^t e^{As}\mathrm{d}s = A^{\#}(e^{At} - I) + (I - AA^{\#})t, t \geqslant 0.$

(vii) $\int_0^t e^{As}\mathrm{d}sP$ *exists iff* $P \in (R)(A)$.

(viii) *If* $P \in (R)(A)$, *then* $\int_0^t e^{As}\mathrm{d}sP = -A^{\#}P$.

(ix) *If* $P \in (R)(A)$ *and* $P \geqslant\geqslant 0$, *then* $-A^{\#}P \geqslant\geqslant 0$.

(x) *A is nonsingular iff -A is a nonsingular M-matrix.*

(xi) *If A is nonsingular, then A is asymptotical stable and* $A^{-1} \leqslant\leqslant 0$.

Proposition 2.1. *Suppose that* $x_0 \geqslant\geqslant 0$ *and* $P \geqslant\geqslant 0$, *then* $x_e := \lim_{t\to\infty} x(t)$ *exists iff* $P \in (R)(A)$ *where* $x_e = (I - AA^{\#})x_0 - A^{\#}P$. *If, in addition, A is nonsingular, then* $x_e = -A^{-1}P$.

Theorem 2.2. *Let A is essentially nonnegative. Then Sys.1 is asymptotically stable iff there exists a positive diagonal matrix P and a positive-definite matrix R s.t.*

$$0 = A^T P + PA + R \tag{3}$$

2.3 stability of nonlinear case

Consider the nonlinear nonnegative dynamical system

$$\dot{x}(t) = f(x(t)), \quad x(0) = x_0, \quad t \in [0, T_{x_0}] \tag{4}$$

where $x(t)\mathcal{D}$, $\mathcal{D}$ is an open subset of $\mathbb{R}^n$ containning $\overline{\mathbb{R}}_+^n$, $f : \mathcal{D} \to \mathbb{R}^n$ is locally Lipschitz. Furthermore, a subset $\mathcal{D}_c \subset \mathcal{D}$ is an invariant set with respect to Sys.4 if $\mathcal{D}_c$ contains the orbits of all its point.

Defination 2.5 (essentially nonnegative vector fields). let $f : \mathcal{D} \to \mathbb{R}^n$. Then f is **essentially nonnegative** if $f_i(x) \geqslant 0$ for all $i = 1, \cdots, n$ and $x \in \overline{\mathbb{R}}_+^n$ s.t. $x_i = 0$.

Proposition 2.2. $\overline{\mathbb{R}}_+^n$ *is an invariant set with respect to Sys.4 iff f is essentially nonnegative.*

Lemma 2.3. *Let* $f(0) = 0$ *and f is essentially nonnegative and continuously differentiable in* $\overline{\mathbb{R}}_+^n$. *Then,* $A := \frac{\partial f}{\partial x}|_{x=0}$ *is essentially nonnegative.*

Theorem 2.3. *Let* $x(t) = x_e$ *be an equilibrium point for Sys.4 and f be essentially nonegative and* $A = \frac{\partial f}{\partial x}|_{x=x_e}$. *Then the following statements hold:*

(i) *If* $Re\lambda < 0$, *where* $\lambda \in spec(A)$, *then the equilibrium solution of the Sys.4 is asymptotically stable.*

(ii) *If there exits* $\lambda \in spec(A)$ *s.t.* $Re\lambda > 0$, *then the equilibrium solution of the Sys.4 is unstable.*

(iii) *Let* $x_e = 0$, $Re\lambda < 0$, *where* $\lambda \in spec(A)$, *let* $p \gg 0$ *be s.t.* $A^T p << 0$, *and define* $\mathcal{D}_A := \{x \in \overline{\mathbb{R}}_+^n : p^T x < \gamma\}$, *where* $\gamma := sup\{\epsilon > 0 : p^T f(x) < 0, \|x\| < \epsilon\}$ *and* $\|x\| = \sum_{i=1}^n p_i x_i$. *Then* $\mathcal{D}_A$ *is a subset of the domain of attraction.*

3 Compartmental Modeling

3.1 General Compartmental Model

Compartment acts like a container which allows mass or energy to flow in and out. It obeys the universial conservation law. Compartments can be interconnected to each other (as seen in Fig.1) and forms compartmetnal dynamic model which is useful in modeling large-scale system. As shown in Fig.1, let $x_i(t), t \geqslant 0, i = 1, \cdots, q$, denotes the mass or energy state (and hence a nonnegative quantity) of the ith compartment, let $\sigma_{ii}(x_i(t)) \geqslant 0$ denote the loss effect of the ith compartment, let $w_i(t) \geqslant 0$ denote the flus supplied to the ith compartment, and let $\phi_{ij}(x)$ denote the net mass flow from the jth compartment to ith compartment which satisfies skew-symmetry constraint $\phi_{ij}(x) = -\phi_{ji}(x)$. Hence, the universal conservation law for the whole system yields a nonlinear comparmental model

$$\dot{x}_i(t) = -\sigma_{ii}(x_i(t)) + \sum_{j=1, j\neq i}^{q} \phi_{ij}(x) + w_i(t), \quad t \geqslant 0, \quad i = 1, \cdots, q \tag{5}$$

Consider the linear case, let $\sigma_{ii}(x_i(t)) = a_{ii}x_i(t)$,$\phi_{ij}(x) = a_{ij}x_j(t) - a_{ji}x_i(t)$, where a_{ii} denotes the loss coefficient and $a_{ij}, i \neq j$ denotes the transfer coefficient, $a_{ij} \geqslant 0$. So the linear compartmental model can be expressed as

$$\dot{x}(t) = Ax(t) + w(t), \quad x(0) = x_0, \quad t \geqslant 0 \tag{6}$$

where $x(t) = [x_1(t), \cdots, x_q(t)]^T, w(t) = [w_1(t), \cdots, w_q(t)]^T$,

$$A_{ij} = \begin{cases} -\sum_{k=1}^{q} a_{ki} & \text{if } i = j \\ a_{ij} & \text{if } i \neq j \end{cases} \tag{7}$$

Note that Eq.7 implies that $\sum_{i=1}^{q} A_{ij} \leqslant 0$. Thus, a compartmental system (with $w(t) \equiv 0$) satisfies

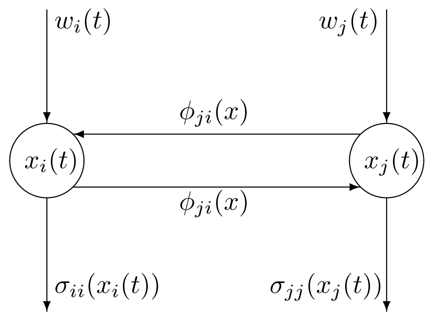

Fig. 1: Compartmental interconnected subsystem model

$\dot{x}_i(t) \leqslant 0$ whenever $x_j(t) = 0, j \neq i$, while a nonnegative system (with $w(t) \equiv 0$) statisfies $\dot{x}_i(t) \geqslant 0$ whenever $x_i(t) = 0$. Note that A is an essentially nonnegative matrix and the Sys.6 is a nonnegative dynamical system. Furthermore, note that $A^Te = [-a_{11}, \cdots, -a_{qq}]^T$, and hence with $p = e = [1, \cdots, 1]^T$ and $r = -A^Te \geqslant\geqslant 0$ it follows that condition (2) is satisfied which implies that the Sys.6 (with $w(t) \equiv 0$) is semistable if A is singular and asymptotically stable if A is nonsingular. In both case, $V(x) = e^Tx = \sum_{i=1}^{q} x_i$ denoting the total mass of the system serves as a Lyapunov function for the undisturbed ($w(t) \equiv 0$) system with $\dot{V} = \sum_{j=1}^{q}(\sum_{i=1}^{q} A_{ij})x_j = -\sum_{i=1}^{q} a_{ii}x_i \leqslant 0, x \in \overline{\mathbb{R}}_+^q$. Alternatively, in the case where $a_{ii} \neq 0$ and $w_i(t) \neq 0$, it follows that Sys.6 cab be equivalently written as

$$\dot{x}(t) = [J_q(x(t)) - D(x(t))] \left(\frac{\partial V}{\partial x}\right)^T + w(t), \quad x(0) = x_0, \quad t \geqslant 0 \tag{8}$$

where $J_q(x)$ is a skew-symmetric matrix function with $J_{q(i,j)} = a_{ij}x_j - a_{ji}x_i$, and $D(x) = \text{diag}[a_{11}x_1, \cdots, a_{qq}x_q]$ $\geqslant\geqslant 0$. Hence, alinear compartmental system is a port-controlled hamiltonian system with a Hamiltonian $V(x)$ representing the total mass, $D(x)$ representing the outflow dissipation, and $w(t)$ representing the supplied flux.

3.2 Interconnected Thermodynamic Systems

To formulate state space thermodynamical model, consider the interconnected dynamical system shown in Fig.1. Let $E_i = x_i$ denote the energy, $S_i = w_i$ denote the external power supplied to or extracted from the subsystem, ϕ_{ij} denote the net instantaneous rate of energy flow from the jth subsystem to ith subsystem, and $\sigma_{ii} = a_{ii}$ denote the instantaneous rate of energy dissipation from the subsystem to environment. An energy balance for each subsystem yields

$$\dot{E}(t) = w(E(t)) - d(E(t)) + S(t), \quad E(t_0) = E_0, \quad t \geqslant t_0 \tag{9}$$

where $w_i(E(t)) = \sum_{j=1,j\neq i}^{q} \phi_{ij}(E)$ and $d_i(E) = \sigma_{ii}(E)$. Since thermodynamic compartmental model involves intercompartmental flows representing energy transfer between compartments, we can use graph-theoretic notions with undirected graph topologies to capture the system interconnections. We define a connectivity matrix $C \in \mathbb{R}^{q\times q}$ s.t. for $i \neq j$, $C_{ij} := 0$ if $\phi_{ij}(E) \equiv 0$ and $C_{ij} := 1$ otherwise, and $C_{ii} := -\sum_{k=1,k\neq i}^{q} C_{ki}$. Recall that if rank$C = q-1$, then system is strongly connected and energy exchange is possible between any two subsystems.

Defination 3.1. A continuously differentiable, strictly concave function $\mathcal{S} : \overline{\mathbb{R}}_+^q \to \mathcal{R}$ is called the entropy function of the system if

$$\left(\frac{\partial \mathcal{S}}{\partial E_i} - \frac{\partial \mathcal{S}}{\partial E_j}\right)\phi_{ij}(E) \geqslant 0, \quad i \neq j \tag{10}$$

and $\frac{\partial \mathcal{S}}{\partial E_i} = \frac{\partial \mathcal{S}}{\partial E_j}$ iff $\phi_{ij}(E) = 0$ with $C_{ij} = 1$.

Proposition 3.1. *Consider the isolated ($S(t) \equiv 0, d(E) \equiv 0$) interconnected dynamical system with the power balance Eq.9. Assume that rank$C = q-1$ and there exists an entropy function $\mathcal{S}$. Then, $\sum_{j=1}^{q} \phi_{ij}(E) = 0$ iff $\frac{\partial \mathcal{S}}{\partial E_i} = \frac{\partial \mathcal{S}}{\partial E_j}$. Furthermore, the set of nonnegative equilibrium states of Eq.9 is given by $\varepsilon_0 := \{E \in \overline{\mathbb{R}}_+^q : \frac{\partial \mathcal{S}}{\partial E_i} = \frac{\partial \mathcal{S}}{\partial E_j}\}$.*

Theorem 3.1. *Consider the isolated ($S(t) \equiv 0, d(E) \equiv 0$) interconnected dynamical system with the power balance Eq.9. Assume that rank$C = q-1$ and there exists an entropy function $\mathcal{S}$. Then, the isolated system is globally semistable with Lyapunov function $V(E) := \mathcal{S}(E_e) - S(E) - \lambda_e(e^T E_e - e^T E)$, where $\lambda_e := \frac{\partial \mathcal{S}}{\partial E_1}(E_e)$ and $E_0 = \frac{1}{q}ee^T E(t_0)$ denotes as the equivalent state.*

In classical thermodynamics, the reciprocal of the system temperature is defined as $T_i := \left(\frac{\partial \mathcal{S}}{\partial E_i}\right)^{-1}$. Eq.10 is a manifestation of the second law of thermodynamics and implies that the energy flows from high temperature subsystem to low temperature one.

4 Vector Dissipativity Theory

Dissipativity theory provides a fundamental framework for the analysis and design of control systems using an input-output desciption based on system energy. The dissipation hypothesis on dynamical systems results in a fundamental constraint on their dynamic behavior wherein a disspative dynamical system can only deliver a fraction of its energy to its surroundings and can only store a fraction of the work done to it. Since complex multi-physical system has numerous input-output properties related to conservation, dissipation, and trasport of mass and energy, it seems natural to extend dissipativity theory to nonnegative and compartmental models which themselves behave in accordance to conservation laws. Specifically, consider the dynamical systems of the from

$$\begin{aligned} \dot{x}(t) &= f(x) + g(x)u, \quad x(0) = x_0, \quad t \geqslant 0 \\ y(t) &= h(x) + j(x)u \end{aligned} \tag{11}$$

Defination 4.1. The Sys.11 is nonnegative if for every $x_0 \in \overline{\mathbb{R}}_+^n$ and $u(t) \geqslant\!\!\geqslant 0$, the solution $x(t)$ and the output $y(t)$ are nonnegative.

Proposition 4.1. *If f is essentially nonnegative, $h(x), g(x), j(x) \geqslant\!\!\geqslant 0, x \in \overline{\mathbb{R}}_+^n$, then Sys.11 is nonnegative.*

Defination 4.2. The Sys.11 is exponentially dissipative (resp., dissipative) with respect to the supply rate $s : \overline{\mathbb{R}}_+^m \times \overline{\mathbb{R}}_+^l \to \mathbb{R}$ if there exists a continuous nonnegative-definite function $V_s : \overline{\mathbb{R}}_+^n \to \overline{\mathbb{R}}_+$ called a storage function and a scalar $\epsilon > 0$ (resp., $\epsilon = 0$) s.t. $V_s(0) = 0$ and the dissipation inequality

$$e^{\epsilon t_2} V_s(x(t_2)) \leqslant e^{\epsilon t_1} V_s(x(t_1)) + \int_{t_1}^{t_2} e^{\epsilon t} s(u(t), y(t))\mathrm{d}t, \quad t_2 \geqslant t_1 \tag{12}$$

If $V_s(\cdot)$ is continuously differentiable, then the dissipation inequality is equivalent to

$$\dot{V}_s(x(t)) + \epsilon V_s(x(t)) \leqslant s(u(t), y(t)), \quad t \geqslant 0 \tag{13}$$

Defination 4.3. A nonnegative dynamical system is zero-state observable if for all $x \in \overline{\mathbb{R}}_+$, $u(t) \equiv 0$ and $y(t) \equiv 0$ implies $x(t) \equiv 0$. A nonnegative dynamical system is reachable if for all $x \in \mathbb{R}_+^n$, there exist a finite time $t_i \leqslant 0$, square integrable input $u(t)$ defined on $[t_i, 0]$, s.t. the state $x(t)$ can be driven from $x(t_i) = 0$ to $x(0) = x_0$.

Theorem 4.1. *The Sys.11 is exponentially dissipative (resp., dissipative) with respect to the supply rate $s(u, y) = q^T y + r^T u$ iff there exists functions $V_s, l, W : \overline{\mathbb{R}}_+^n \to \overline{\mathbb{R}}_+$, and a scalar $\epsilon > 0$ (resp., $\epsilon = 0$) s.t. $V_s(\cdot)$ is continuously differentiable, $V_s(0) = 0$, and for all $x \in \overline{\mathbb{R}}_+^n$,*

$$
\begin{aligned}
0 &= V_s'(x)f(x) + \epsilon V_s(x) - q^T h(x) + l(x) \\
0 &= V_s'(x)g(x) - q^T j(x) - r^T + W^T(x)
\end{aligned}
\tag{14}
$$

We begin by considering the nonnegative dynamical system with the nonlinear nonegative dynamical feedback system given by

$$
\begin{aligned}
\dot{x}_c(t) &= f_c(x_c(t)) + g_c(x_c(t))u_c(t), \quad x_c(0) = x_{c0}, \quad t \geqslant 0 \\
y_c(t) &= h_c(x_c(t))
\end{aligned}
\tag{15}
$$

where f_c is essentially nonnegative, $g_c(x_c), h_c(x_c) \geqslant\geqslant 0$.

Theorem 4.2. *Consider the Sys.11 and Sys.15, assume Sys.11 is dissipative with respect to the linear supply rate $s(u, y) = q^T y + r^T u$ and with a positive-definite storage function $V_s(\cdot)$, and assume that Sys.15 is dissipative with respect to the linear supply rate $s_c(u_c, y_c) = q_c^T y_c + r_c^T u_c$ and with a positive-definite storage function $V_{sc}(\cdot)$. Then the following statements hold:*

(i) If there exists a scalar $\sigma > 0$ s.t. $q + \sigma q_c \leqslant\leqslant 0$ and $r + \sigma q_c \leqslant\leqslant 0$, then the positive feedback interconnection is Lyapunove stable.

(ii) If these two systems are zero-stable observable and there exists a scalar $\sigma > 0$ s.t. $q + \sigma r_c << 0$ and $r + \sigma q_c << 0$, then the positive feedback interconnection is asympototically stable.

(iii) If Sys.11 is zero-state observable and Sys.15 is exponentially dissipative, and there exists a scalar $\sigma > 0$ s.t. $q + \sigma q_c \leqslant\leqslant 0$ and $r + \sigma q_c \leqslant\leqslant 0$, then the positive feedback interconnection is asympototically stable.

(iv) If Sys.11 is exponentially dissipative, Sys.15 is exponentially dissipative and there exists a scalar $\sigma > 0$ s.t. $q + \sigma q_c \leqslant\leqslant 0$ and $r + \sigma q_c \leqslant\leqslant 0$, then the positive feedback interconnection is asympototically stable.

Consider the feedback nonnegative time-varying input nonlinearity $\sigma(\cdot, \cdot) \in \Phi$,where

$$
\begin{aligned}
\Phi := &\{\sigma : \overline{\mathbb{R}}_+ \times \overline{\mathbb{R}}_+^l \to \overline{\mathbb{R}}_+^m : \sigma(., 0) = 0,\ 0 \geqslant\geqslant \sigma(t, y) \geqslant\geqslant My,\ y \in \overline{\mathbb{R}}_+^l, \\
&\text{a.e. } t \geqslant 0, \text{ and } \sigma(\cdot, y) \text{ is Lebesgue measurable,, } M >> 0\}
\end{aligned}
\tag{16}
$$

Theorem 4.3. *Consider Sys.11 is zero-state observable and exponentially dissipative with respect to the supply rate $s(u, y) = e^T u - e^T My$, where $M >> 0$. Then the positive feedback interconnection of Sys.11 and $\sigma(\cdot, \cdot)$ is globally asymptotically stable.*

5 Application in Chemical Process Control

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