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 future applications in chemical process control.

Contents

1 Introduction . . . 1
2 Nonnegative Dynamics . . . 1
2.1 Mathematical Preliminaries . . . 1
2.2 Stability of linear case . . . 2
2.3 stability of nonlinear case . . . 3
3 Compartmental Modeling . . . 4
3.1 General Compartmental Model . . . 4
3.2 Interconnected Thermodynamic Systems . . . 5
3.3 Gibbs and Helmoholtz Free Energy . . . 5
3.4 Chemical Potential . . . 6
4 Vector Dissipativity Theory . . . 7
4.1 Generalized Vector Dissipativity . . . 8
4.2 Thermodynamics and Vector Dissipativity . . . 10
5 Future Application in Chemical Process Control . . . 10

1 Introduction

Chemical process dynamics involves mass recycle and heat intergration. Traditionally, the model is based on state space with interaction modeled 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 aspects of thermodynamics, including its fundamental laws. So maybe, the compartmental modeling would be an alternative solution to the plant-wide complexity of chemical process. And the control approach 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 nonnegative (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*$\lambda \geq 0$, $\lambda \in \mathrm{spec}(A)$.

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

Furthermore, in the case where A is a nonsingular 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 nonnegative 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 equilibrium 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* $\lambda \in \mathrm{spec}(A)$, *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 nonsigular 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 $\mathbb{R}^n$ containing $\overline{\mathbb{R}}^n_+$, $f : \mathcal{D} \to \mathbb{R}^n$ 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 nonnegative 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 universal 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

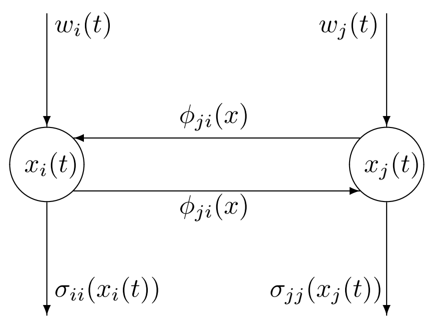

Fig. 1: Compartmental interconnected subsystem model

$\dot{x}_i(t) \leqslant 0$ whenever $x_j(t) = 0, j \neq i$, while a nonnegative system (with $w(t) \equiv 0$) satisfies $\dot{x}_i(t) \geqslant 0$ 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 $A^T e = [-a_{11}, \cdots, -a_{qq}]^T$, and hence with $p = e = [1, \cdots, 1]^T$ and $r = -A^T e \geqslant\geqslant 0$ 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, $V(x) = e^T x = \sum_{i=1}^{q} x_i$ 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, a linear 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 $E_e = \frac{1}{q} e e^T E(t_0)$ 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.

3.3 Gibbs and Helmoholtz Free Energy

According to the classical thermodynamics, an additional (deformation) state representing subsystem volumes in order to introduce the notion of work into our thermodynamically consistent state space energy flow model. The rate of work done by the subsystem to environment is denoted by d_{wi}, the rate of work done by its environment is denoted by S_{wi}, the volume of the subsystem is V_i and the pressure $p_i(E, V)$. The net work done by each subsystem on the environment satisfies

$$p_i(E, V)\mathrm{d}V_i = (d_{wi}(E, V) - S_{wi}(t)\mathrm{d}t \tag{11}$$

The definition of entropy in the presence of work remains the same as in Definition 3.1 with $\mathcal{S}(E)$ replaced by $\mathcal{S}(E, V)$. Note that

$$\frac{\mathrm{d}\mathcal{S}}{\mathrm{d}t} = \frac{\partial \mathcal{S}}{\partial E_i}\frac{\mathrm{d}E_i}{\mathrm{d}t} + \frac{\partial \mathcal{S}}{\partial V_i}\frac{\mathrm{d}V_i}{\mathrm{d}t} \tag{12}$$

$$p_i(E, V) = \left(\frac{\partial \mathcal{S}}{\partial E_i}\right)^{-1}\left(\frac{\partial \mathcal{S}}{\partial V_i}\right) \tag{13}$$

In the presence of work energy, the power balance Eq.9 takes the new form involving energy and deformation states

$$\dot{E} = w(E,V) - d_w(E,V) + S_w(t) - d(E,V) + S(t) \tag{14}$$
$$\dot{V} = D(E,V)(d_w(E,V) - S_w(t)) \tag{15}$$

where $D(E,V) := \text{diag}\left[\left(\frac{\partial\mathcal{S}}{\partial E_i}\right)^{-1}\left(\frac{\partial\mathcal{S}}{\partial V_i}\right)\right]$ and $\left(\frac{\partial\mathcal{S}}{\partial V}\right)D(E,V) = \left(\frac{\partial\mathcal{S}}{\partial E}\right)$. Then the fundamental law of thermodynamics can be developed from Eq.(14,15)

$$\text{First Law:} \quad \delta U = \mathrm{d}Q - \mathrm{d}W \tag{16}$$
$$\text{Second Law:} \quad \mathrm{d}\mathcal{S} \geqslant \sum_{i=1}^{q} \frac{\mathrm{d}Q_i}{\mathrm{d}T_i} \tag{17}$$

Next, we define the Gibbs free energy, the Helmholtz free energy, and the enthalpy functions for the interconnected dynamical system. The Gibbs free energy is defined by

$$G(E,V) := e^T E - \sum_{i=1}^{q}\left(\frac{\partial\mathcal{S}}{\partial E_i}\right)^{-1}\mathcal{S}_i(E_i,V_i) + \sum_{i=1}^{q}\left(\frac{\partial\mathcal{S}}{\partial E_i}\right)^{-1}\left(\frac{\partial\mathcal{S}}{\partial V_i}\right)V_i \tag{18}$$

the Helmholtz free energy is defined by

$$F(E,V) := e^T E - \sum_{i=1}^{q}\left(\frac{\partial\mathcal{S}}{\partial E_i}\right)^{-1}\mathcal{S}_i(E_i,V_i) \tag{19}$$

and the enthalpy is defined by

$$H(E,V) := e^T E + \sum_{i=1}^{q}\left(\frac{\partial\mathcal{S}}{\partial E_i}\right)^{-1}\left(\frac{\partial\mathcal{S}}{\partial V_i}\right)V_i \tag{20}$$

Note that the above definitions are consistent with the classical thermodynamic difinitions given by $G(E,V) = U + pV - TS$, $F(E,V) = U - TS$, and $H(E,V) = U + pV$.

3.4 Chemical Potential

In chemical reaction, an additional mass balance is included for addressing conservation of energy as well as conservation of mass. This additional mass conservation equation would involve the law of mass-action enforce proportionality between a particular reaction rate and the concentrations of the reactants. Consider chemical reaction networks described by

$$\sum_{j=1}^{q} A_{ij}X_j \xrightarrow{k_i} \sum_{j=1}^{q} B_{ij}X_j \tag{21}$$

where A_{ij}, B_{ij} are the stoichiometric coefficients and k_i denotes the reaction rate. It can be written in a compactly in matrix-vector form as

$$AX \xrightarrow{k} BX \tag{22}$$

Let n_j denote the mole number of the jth species. Invoking the law of mass-action, a reaction in which all of the stoichiometric coefficients of the reactants are one, the rate of reaction is proportional to the product of the concentrations of the reactants, the species quantities change

$$\dot{n}(t) = (B-A)^T K n^A(t), \quad n(0) = n_0, \quad t \geqslant t_0 \tag{23}$$

where $K := \text{diag}[k_1, \cdots, k_r]$ and $n^A := \left[\Pi_{j=1}^{q} n_j^{A_{1j}}, \cdots, \Pi_{j=1}^{q} n_j^{A_{rj}}\right]^T$. Furthermore, let $M_j > 0$ denote the molar mass of the jth species, let $m_j = M_j n_j$ denote the mass of the jth species. Then, using the transformation $m(t) = Mn(t)$ where $M := \mathrm{diag}[M_1, \cdots, M_q]$, the mole balance equation can be rewritten as the mass balance

$$\dot{m}(t) = M(B-A)^T \tilde{K} m^A(t) \tag{24}$$

where $\tilde{K} := \mathrm{diag}\left[\frac{k_1}{\Pi_{j=1}^q M_j^{A_{1j}}}, \cdots, \frac{k_1}{\Pi_{j=1}^q M_j^{A_{rj}}}\right]$. In the absence of nuclear reactions, the total mass of the species during each reaction is conserved

$$e^T M(B-A)^T = 0 \tag{25}$$

The chemical potential has a strong connection with the second law of thermodynamics in that every process in nature evolves from a state of higher chemical potential towards a state of lower chemical potential. It was postulated by Gibbs that the change in energy of a homogeneous substance is proportional to the change in mass of this substance with the coefficient of proportionality given by the chemical potential of the substance.

$$\dot{E} = w(E) + P(E,m)M(B-A)^T \tilde{K} m^A(t) - d(E) + S(t) \tag{26}$$

$$\dot{m} = M(B-A)^T \tilde{K} m^A(t) \tag{27}$$

where $P(E,m) := \mathrm{diag}\left[\mu_1(E,m), \cdots, \mu_q(E,m)\right]$ and $\mu_i(\cdot,\cdot)$ is the chemical potential of a unit mass. We assume that if $E_j = 0$, then $\mu_j(E,m) = 0$.

Note. For the chemical reaction network with mass balance, assume that $\mu(E,m) >> 0$ for all $E \neq 0$ and

$$\nu(E,m) = (A-B)M\mu(E,m) \geqslant\geqslant 0 \tag{28}$$

where $\mu(E,m)$ is the vector of chemical potential of the substance and $\nu(E,m)$ is the affinity vector.

4 Vector Dissipativity Theory

Dissipativity theory provides a fundamental framework for the analysis and design of control systems using an input-output description 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 transport 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 form

$$\begin{aligned} \dot{x}(t) &= f(x) + g(x)u, \quad x(0) = x_0, \quad t \geqslant 0 \\ y(t) &= h(x) + j(x)u \end{aligned} \tag{29}$$

Defination 4.1. The Sys.29 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.29 is nonnegative.*

Defination 4.2. The Sys.29 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

$$e^{\epsilon t_2} V_s(x(t_2)) \leqslant e^{\epsilon t_1} V_s(x(t_1)) + \int_{t_1}^{t_2} e^{\epsilon t} s(u(t), y(t)) \mathrm{d}t, \quad t_2 \geqslant t_1 \tag{30}$$

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

$$\dot{V}_s(x(t)) + \epsilon V_s(x(t)) \leqslant s(u(t), y(t)), \quad t \geqslant 0 \tag{31}$$

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.29 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 $x \in \overline{\mathbb{R}}^n_+$,*

$$\begin{aligned} 0 &= V_s'(x) f(x) + \epsilon V_s(x) - q^T h(x) + l(x) \\ 0 &= V_s'(x) g(x) - q^T j(x) - r^T + W^T(x) \end{aligned} \tag{32}$$

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

$$\begin{aligned} \dot{x}_c(t) &= f_c(x_c(t)) + g_c(x_c(t)) u_c(t), \quad x_c(0) = x_{c0}, \quad t \geqslant 0 \\ y_c(t) &= h_c(x_c(t)) \end{aligned} \tag{33}$$

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

Theorem 4.2. *Consider the Sys.29 and Sys.33, assume Sys.29 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.33 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.29 is zero-state observable and Sys.33 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.29 is exponentially dissipative, Sys.33 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

$$\begin{aligned} \Phi := &\{\sigma : \overline{\mathbb{R}}_+ \times \overline{\mathbb{R}}^l_+ \to \overline{\mathbb{R}}^m_+ : \sigma(.,0) = 0,\ 0 \geqslant\geqslant \sigma(t, y) \geqslant\geqslant My,\ y \in \overline{\mathbb{R}}^l_+, \\ &\text{a.e. } t \geqslant 0, \text{ and } \sigma(\cdot, y) \text{ is Lebesgue measurable,}, M >> 0\} \end{aligned} \tag{34}$$

Theorem 4.3. *Consider Sys.29 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.29 and $\sigma(\cdot, \cdot)$ is globally asymptotically stable.*

4.1 Generalized Vector Dissipativity

We extend the notion of dissipative dynamical systems to develop the generalized notion of vector dissipativity for large-scale nonlinear dynamical systems. Consider the large-scale nonlinear dynamical systems of the form

$$\dot{x}(t) = F(x(t), u(t)) \tag{35}$$

$$y(t) = H(x(t), u(t)) \tag{36}$$

where $x \in \mathcal{D} \subset \mathbb{R}^n$,$u \in \mathcal{U} \subset \mathbb{R}^m$, $y \in \mathcal{Y} \subset \mathbb{R}^l$,$F : \mathcal{D} \times \mathcal{U} \to \mathbb{R}^n$, $H : \mathcal{D} \times \mathcal{U} \to \mathcal{Y}$, $F(0, 0) = 0$. Here, assume that it represents a large-scale dynamical system composed of q interconnected subsystems

$$F_i(x, u_i) = f_i(x_i) + I_i(x) + G_i(x_i) u_i \tag{37}$$

$$H_i(x_i, u_i) = h_i(x_i) + J_i(x_i) u_i \tag{38}$$

Defination 4.4. The Sys.35 is vector dissipative with respect to the vector supply rate $S(u,y)$ if there exists a continuous, nonnegative definite vector function V_s, called a vector storage function, and an essentially nonnegative dissipation matrix W s.t $V_s(0) = 0$, W is semistable, and the vector dissipation inequality is satisfied.

$$V_s(x(T)) \leqslant\leqslant e^{W(T-t_0)} V_s(x(t_0)) + \int_{t_0}^{T} e^{W(T-t)} S(u(t), y(t)) \mathrm{d}t \tag{39}$$

And define the vector available storage of the large-scale system by

$$V_a(x_0) := \sup_{T \geqslant t_0, u(\cdot)} \left[-\int_{t_0}^{T} e^{-W(t-t_0)} S(u(t), y(t)) \mathrm{d}t \right] \tag{40}$$

where $x(t_0) = x_0$. And the concept of vector required supply is defined by

$$V_r(x_0) := \inf_{T \geqslant -t_0, u(\cdot)} \left[\int_{-T}^{t_0} e^{-W(t-t_0)} S(u(t), y(t)) \mathrm{d}t \right] \tag{41}$$

where $x(-T) = 0, x_(t_0) = x_0$.

Lemma 4.1. *The system is vector dissipative with respect to the vector supply rate $S(u,y)$ iff*

$$\dot{V}_s(x(t)) \leqslant\leqslant W V_s(x(t)) + S(u(t), y(t)) \tag{42}$$

Lemma 4.2. *Assume each disconnected subsystem is exponentially dissipative with respect to supply rate $s_i(u_i, y_i)$ and with a continuously differential storage function v_{si}. Furthermore, assume that the interconnection functions $I_i : \mathcal{D} \to \mathbb{R}^{n_i}$ art s.t.*

$$v'_{si}(x_i) I_i(x) \leqslant \sum_{j=1}^{q} \xi_{ij}(x) v_{sj}(x_j) \tag{43}$$

where ξ_{ij} are bounded functions. If W is semistable with

$$W_{ij} = \begin{cases} -\varepsilon_i + \alpha_{ii} & \text{if } i = j \\ \alpha_{ij} & \text{if } i \neq j \end{cases} \tag{44}$$

where $\varepsilon_i > 0$ and $\alpha_{ij} := max\{0, \sup_{x \in \mathcal{D}} \xi_{ij}(x)\}$. Then the large-scale system is vector dissipativity.

Theorem 4.4. *Consider the large-scale system with S, W, then*

$$\int_{t_0}^{T} e^{W(t-t_0)} S(u(t), y(t)) \, dt \geqslant\geqslant 0 \tag{45}$$

for $x(t_0) = 0$ iff $V_a(0) = 0$ and $V_a(x)$ is finite. Moreover, if (45) holds, then $V_a(x)$ is a vector storage function.

Theorem 4.5. *Assume the system completely reachable, then it is vector dissipative with respect to the vector supply rate $S(u,y)$ iff*

$$0 \leqslant\leqslant V_r(x) \leqslant\leqslant \infty \tag{46}$$

Moreover, if (46) holds, then $V_r(x)$ is a vector storage function. Finally, if $V_a(x)$ is a vector available storage function, then

$$0 \leqslant\leqslant V_a(x) \leqslant\leqslant V_s(x) \leqslant\leqslant V_r(x) \leqslant\leqslant \infty \tag{47}$$

And let $M = diag[\mu_1, \cdots, \mu_q], 0 \leqslant \mu_i \leqslant 1$, then every vector storage function has the form

$$V_s(x) = M V_a(x) + (I_q - M) V_r(x) \tag{48}$$

Theorem 4.6. *Consider the system which zero-state observable and vector dissipative. Furthermore, assume W has an non-positive eigenvalue $-\alpha$ and positive vector p. In addition, assume that there exist function $k_i : \mathcal{Y}_i \to \mathcal{U}_i$ s.t. $k_i(0) = 0$ and $S_i(k_i(y_i), y_i) < 0$. Then for all vector storage function V_s the global storage function $v_s(x) := p^T V_s(x)$ is positive definite.*

4.2 Thermodynamics and Vector Dissipativity

The fundamental and unifying concept in the analysis and control design of large-scale systems is the concept of energy. The energy of a state of a dynamical system is the measure of its ability to produce changes in its own state as well as changes in the system states of its surroundings. As in thermodynamic systems, dynamical systems exhibit energy that becomes unavailable to do useful work.

5 Future Application in Chemical Process Control

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