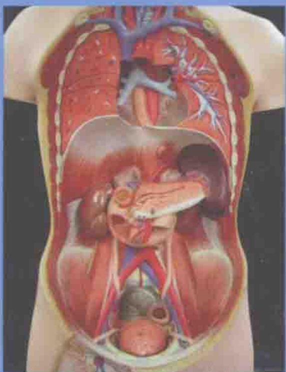

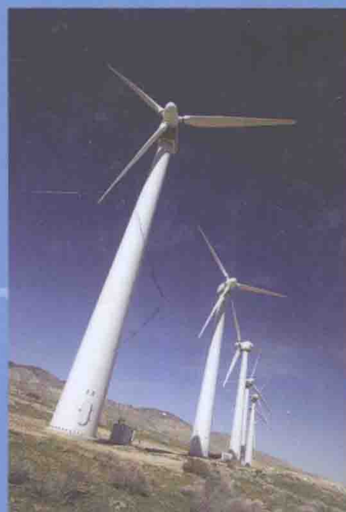

Nonnegative and Compartmental Dynamical Systems

Wassim M. Haddad, VijaySekhar Chellaboina, and Qing Hui

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Preface

Nonnegative and compartmental dynamical system models are derived from mass and energy balance considerations that involve dynamic states whose values are nonnegative. These models are widespread in biology, chemistry, ecology, economics, genetics, medicine, sociology, and engineering, and play a key role in the understanding of these disciplines. Specifically, since such disciplines give rise to systems that have numerous input, state, and output properties related to conservation, dissipation, and transport of mass and energy, nonnegative and compartmental models are conceptually simple yet remarkably effective in describing the essential phenomenological features of these dynamical systems. Furthermore, since such systems are governed by conservation laws (e.g., mass, energy, fluid, etc.) and are comprised of homogeneous compartments which exchange variable nonnegative quantities of material via intercompartmental flow laws, these systems are completely analogous to network thermodynamic (advection-diffusion) systems with compartmental masses or energies playing the role of heat and temperatures.

Compartmental models have been widely used in biology, pharmacology, and physiology to describe the distribution of a substance (e.g., biomass, drug, radioactive tracer, etc.) among different tissues of an organism. In this case, a compartment represents the amount of the substance inside a particular tissue and the intercompartmental flows are due to diffusion processes. In engineering and the physical sciences, compartments typically represent the energy, mass, or information content of the different parts of the system, and different compartments interact by exchanging heat, work energy, and matter. In ecology and economics, compartments can represent soil and debris, or finished goods and raw materials in different regions, and the flows are due to energy and nutrient exchange (e.g., nitrates, phosphates, carbon, etc.), or money and securities. Compartmental systems can also be used to model chemical reaction systems. In this case, the compartments would represent quantities of different chemical substances contained within the compartment, and the compartmental flows would characterize transformation rates of reactants to products.

In this monograph, we develop a unified stability and dissipativity (i.e., conservation, dissipation, and transport) analysis and control design framework for nonnegative and compartmental dynamical systems in order to foster the understanding of these systems as well as advancing the state of the art in active control of nonnegative and compartmental systems. This general framework is then applied to the fields of thermal sciences, biology, chemistry, and medicine to provide a dynamical systems perspective of these diverse disciplines. The monograph is written from a system-theoretic point of view and can be viewed as a contribution to dynamical system and control system theory.

After a brief introduction to nonnegative and compartmental dynamical systems in Chapter 1, fundamental stability theory for linear and nonlinear nonnegative and compartmental dynamical systems is developed in Chapter 2. In Chapter 3, we extend the results of Chapter 2 to address nonnegative and compartmental systems with time delay. Chapter 4 provides necessary and sufficient conditions for identifying nonnegative and compartmental systems that admit nonoscillatory and monotonic solutions. A detailed treatment of dissipativity theory and stability of feedback interconnections of nonnegative dynamical systems is given in Chapter 5, whereas extensions of these results to impulsive nonnegative systems are given in Chapter 6. In Chapters 7 and 8 we use compartmental dynamical system theory to provide a system-theoretic foundation for thermodynamics. A detailed treatment of mass-action kinetics is given in Chapter 9, while Chapters 10 and 11 provide extensions to general compartmental models with directed and undirected intercompartmental flows, time delays, and model uncertainty. Next, in Chapters 12–16 we develop a control design framework for nonnegative and compartmental dynamical systems with application to drug dosing control for clinical pharmacology. In Chapter 17, we use compartmental dynamical system theory and Poincaré maps to model, analyze, and control the dynamics of a pressure-limited respirator and lung mechanics system. Chapter 18 develops a constrained optimization framework for nonnegative and compartmental system identification. Finally, in Chapter 19 we present conclusions.

The first author would like to thank James M. Bailey for his valuable discussions on pharmacokinetic and pharmacodynamic modeling in clinical pharmacology over the recent years. In addition, the authors thank Paul Katinas for several insightful and enlightening discussions on the statements quoted in ancient Greek on page vii. In some parts of the monograph we have relied on work we have done jointly with Elias August, James M. Bailey, Dennis S. Bernstein, Sanjay P. Bhat, Behnood Gholami, Tomohisa Hayakawa, Hancao Li, Sergey G. Nersesov, Tanmay Rajpurohit, Jayanthy Ramakrishnan, and Kostyantyn Y. Volyanskyy; it is a pleasure to acknowledge their contributions.

The aphorisms by Herakleitos, Empedocles, and Pythagoras quoted in the epigraph of the book give the earliest perception of the complexity of nature and universe. For example, biology has shown that many species of animals such as insect swarms, ungulate flocks, fish schools, ant colonies, and bacterial colonies self-organize in nature. These biological aggregations give rise to remarkably complex global behaviors from simple local interactions between a large number of relatively unintelligent agents without the need for a centralized architecture. The spontaneous development (i.e., self-organization) of these autonomous biological systems and their spatio-temporal evolution to more complex states often appears without any external system interaction. In other words, structural morphing into coherent groups is internal to the system and results from local interactions among subsystem components that are independent of the physical nature of the individual components. These local interactions often comprise a simple set of rules that lead to remarkably complex and robust behaviors. Complexity here refers to the quality of a system wherein interacting subsystems self-organize to form hierarchical evolving structures exhibiting emergent system properties, whereas robustness refers to insensitivity of individual subsystem failures and unplanned behavior at the individual subsystem level. The connection between the local subsystem interactions and the globally complex system behavior is often elusive. This is true for nature in general and was most eloquently stated first by the ancient Greek philosopher Herakleitos in his 123rd fragment—Nature loves to hide (Φύσις κρύπτεσθαι φιλεί).

Herakleitos' profound second statement—All matter is exchanged for energy, and energy for all matter (Πυρός τε ἀνταμοιβὴ τὰ πάντα καὶ πῦρ ἁπάντων)—is a statement of the law of conservation of mass-energy and is a precursor to the principle of relativity. In describing the nature of the universe Herakleitos postulates that nothing can be created out of nothing, and nothing that disappears ceases to exist. This totality of forms, or mass-energy equivalence, is eternal and unchangeable in a constantly changing universe (τα πάυτα ρεί). Herakleitos' last statement defines ultimate wisdom as knowledge and understanding of the intelligence which steers all things through all things. In the language of modern science, this statement defines ultimate wisdom as a fundamental understanding of the universal laws that govern all things and all forces in the universe.

Like Herakleitos' second statement, Empedocles' statement is one of totality of forms in nature. He postulates that there is no genesis with regard to any of the things in nature but rather a blending and alteration of elements (στοιχεία) through attractive and repulsive forces. He further postulates that the organic universe originated from spontaneous aggregations involving pattern interactions by which life emerged through autopoiesis (self-creation). Pythagoras' statement attempting to explain our incomprehensible universe is as trenchant today as it was two and a half millennia ago, with parts of his statement resonating with creationists, evolution theorists, and intelligent designers. However, Pythagoras spoke of one god, and of God in many forms, and he did so without contradiction. And with God elicited as the universal forces (strong nuclear, electromagnetic, weak nuclear, and gravitational), his statement belongs to the scientist.

The results reported in this monograph were obtained at the School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, and the Department of Mechanical, Aerospace, and Biomedical Engineering of the University of Tennessee, Knoxville, between June 2000 and May 2008. The research support provided by the Air Force Office of Scientific Research and the National Science Foundation over the years has been instrumental in allowing us to explore basic research topics that have led to some of the material in this monograph. We are indebted to them for their support.

Atlanta, Georgia, USA, July 2009, *Wassim M. Haddad*

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Chapter One

Introduction

With the ever-increasing influence of mathematical modeling and engineering on biological, social, and medical sciences, it is not surprising that dynamical system theory has played a central role in the understanding of many biological, ecological, and physiological processes [155, 171, 172, 235]. With this confluence it has rapidly become apparent that mathematical modeling and dynamical system theory are the key threads that tie together these diverse disciplines. The dynamical models of many biological, pharmacological, and physiological processes such as pharmacokinetics [19, 287], metabolic systems [50], epidemic dynamics [155, 157], biochemical reactions [57, 171], endocrine systems [50], and lipoprotein kinetics [171] are derived from mass and energy balance considerations that involve dynamic states whose values are nonnegative. Hence, it follows from physical considerations that the state trajectory of such systems remains in the nonnegative orthant of the state space for nonnegative initial conditions. Such systems are commonly referred to as *nonnegative dynamical systems*[1] in the literature [79, 164, 166, 233].

A subclass of nonnegative dynamical systems are *compartmental systems* [4, 5, 29, 43, 88, 100, 134, 152, 155–158, 162, 165, 188, 198, 208, 209, 211, 219, 220, 232, 252, 258, 259, 300]. Compartmental systems involve dynamical models that are characterized by conservation laws (e.g., mass, energy, fluid, etc.) capturing the exchange of material between coupled macroscopic subsystems known as *compartments*. Each compartment is assumed to be kinetically homogeneous, that is, any material entering the compartment is instantaneously mixed with the material of the compartment. The range of applications of nonnegative systems and compartmental systems is not limited to biological, social, and medical systems. Their usage includes chemical reaction systems [25, 60, 82, 187, 298], queuing systems [301], large-scale systems [274, 275], stochastic systems (whose state variables

[1]Some authors erroneously refer to nonnegative dynamical systems as *positive systems*. However, since the state of a nonnegative system can evolve in the nonnegative (closed) orthant of the state space, which is a *proper cone* (i.e., a closed, convex, solid, and pointed cone), and is not necessarily constrained to the positive (open) orthant of the state space, *nonnegative dynamical systems* is the appropriate expression for the description of such systems.

represent probabilities) [301], ecological systems [38, 141, 181, 211, 231], economic systems [21], demographic systems [155], telecommunications systems [90], transportation systems, power systems, heat transfer systems, thermodynamic systems [116], and structural vibration systems [175–177], to cite but a few examples.

In economic systems the interaction of raw materials, finished goods, and financial resources can be modeled by compartments representing various interacting sectors in a dynamic economy. Similarly, network systems, computer networks, and telecommunications systems are all amenable to compartmental modeling with intercompartmental flow laws governed by nodal dynamics and rerouting strategies that can be controlled to minimize waiting times and optimize system throughput. Compartmental models can also be used to model the interconnecting components of power grid systems with energy flow between regional distribution points subject to control and possible failure. Road, rail, air, and space transport systems also give rise to compartmental systems with interconnections subject to failure and real-time modification.

Since the aforementioned dynamical systems have numerous input, state, and output properties related to conservation, dissipation, and transport of mass, energy, or information, nonnegative and compartmental models are conceptually simple yet remarkably effective in describing the essential phenomenological features of these dynamical systems. Furthermore, since such systems are governed by conservation laws and are comprised of homogeneous compartments which exchange variable nonnegative quantities of material via intercompartmental flow laws, these systems are completely analogous to network thermodynamic (advection-diffusion) systems with compartmental masses, energies, or information playing the role of heat and temperatures.

The goal of the present monograph is directed toward developing a general stability[2] analysis and control design framework for nonlinear nonnegative and compartmental dynamical systems. However, as in general nonlinear systems, nonlinear nonnegative dynamical systems can exhibit a very rich dynamical behavior, such as multiple equilibria, limit cycles, bifurcations, jump resonance phenomena, and chaos, which can make general nonlinear nonnegative system analysis and control notoriously difficult. In addition, since nonnegative and compartmental dynamical systems have specialized structures, nonlinear nonnegative system stabilization has received very little attention in the literature and remains

[2]Unlike standard stability theory, stability notions for nonnegative dynamical systems need to be defined with respect to *relatively open* subsets of the nonnegative orthant of the state space containing the system equilibrium point. See Definition 2.3.

relatively undeveloped. For example, biological and physiological systems typically possess a multiechelon hierarchical hybrid structure characterized by continuous-time dynamics at the lower levels of the hierarchy and discrete-time dynamics (logical decision-making units) at the higher levels of the hierarchy. This is evident in all living systems wherein control structures and hierarchies are present at the intracellular level, the intercellular level, the organs, and the organ system and organism level. Furthermore, biological and physiological systems are self-regulating systems, and hence, they additionally involve feedback (nested or interconnected) subsystems within their hierarchical structures. Finally, the complexity of biological and physiological system modeling and control is further exacerbated when addressing system modeling uncertainty inherent to system biology and physiology.

Another complicating factor in the stability analysis of many nonnegative and compartmental dynamical systems is that these systems possess a continuum of equilibria. Since every neighborhood of a nonisolated equilibrium contains another equilibrium, a nonisolated equilibrium cannot be asymptotically stable. Hence, asymptotic stability is not the appropriate notion of stability for systems having a continuum of equilibria. Two notions that are of particular relevance to such systems are *convergence* and *semistability*. Convergence is the property whereby every system solution converges to a limit point that may depend on the system initial condition. Semistability is the additional requirement that all solutions converge to limit points that are Lyapunov stable. Semistability for an equilibrium thus implies Lyapunov stability, and is implied by asymptotic stability.[3] The dependence of the limiting state on the initial state is seen in numerous stable nonnegative systems and compartmental systems. For these systems, every trajectory that starts in a neighborhood of a Lyapunov stable equilibrium converges to a (possibly different) Lyapunov stable equilibrium, and hence, these systems are semistable.

The main objective of this monograph is to develop a general analysis and control design framework for nonnegative and compartmental dynamical systems. The main contents of the monograph are as follows. In Chapter 2, we establish notation and definitions, and develop stability theory for nonnegative and compartmental dynamical systems. Specifically, Lyapunov stability theorems as well as invariant set stability theorems are developed for linear and nonlinear, continuous-time and discrete-time nonnegative and compartmental dynamical systems. Chapter 3 provides an extension of the results of Chapter 2 to nonnegative and compartmental dynamical systems

[3]It is important to note that semistability is not merely equivalent to asymptotic stability of the set of equilibria. Indeed, it is possible for a trajectory to converge to the set of equilibria without converging to any one equilibrium point as examples in [34] show.

with time delay. Specifically, stability theorems for linear and nonlinear nonnegative and compartmental dynamical systems with time delay are established using Lyapunov-Krasovskii functionals.

Since nonlinear nonnegative and compartmental dynamical systems can exhibit a full range of nonlinear behavior, including bifurcations, limit cycles, and even chaos, in Chapter 4 we present necessary and sufficient conditions for identifying nonnegative and compartmental systems that admit only nonoscillatory and monotonic solutions. As a result, we provide sufficient conditions for the absence of limit cycles in nonlinear compartmental systems.

In Chapter 5, using generalized notions of system mass and energy storage, and external flux and energy supply, we present a systematic treatment of dissipativity theory for nonnegative and compartmental dynamical systems. Specifically, using linear and nonlinear storage functions with linear supply rates, we develop new notions of dissipativity theory for nonnegative dynamical systems. In addition, we develop new Kalman-Yakubovich-Popov equations for nonnegative systems for characterizing dissipativeness with linear and nonlinear storage functions and linear supply rates. Finally, these results are used to develop general stability criteria for feedback interconnections of nonnegative dynamical systems. In Chapter 6, we extend the results of Chapters 2 and 5 to develop stability and dissipativity results for impulsive nonnegative and compartmental dynamical systems.

Using the concepts developed in Chapters 2, 4, and 5, in Chapter 7 we use compartmental dynamical system theory to provide a system-theoretic foundation for thermodynamics. Specifically, using a state space formulation, we develop a nonlinear compartmental dynamical system model characterized by energy conservation laws that are consistent with basic thermodynamic principles. In addition, we establish the existence of a unique, continuously differentiable global entropy function for our compartmental thermodynamic model, and using Lyapunov stability theory we show that the proposed thermodynamic model has convergent trajectories to Lyapunov stable equilibria with a uniform energy distribution determined by the system initial energies. Finally, using the system entropy, we establish the absence of Poincaré recurrence for our thermodynamic model and develop a clear connection between irreversibility, the second law of thermodynamics, and the entropic arrow of time.

In Chapter 8, we merge the theories of semistability and finite-time stability [32, 35] to develop a rigorous framework for finite-time thermodynamics. Specifically, using a geometric description of homogeneity theory, we develop intercompartmental flow laws that guarantee finite-time