
OFFICE OF NAVAL RESEARCH
FINAL REPORT
PUBLICATIONS/PATENTS/PRESENTATIONS/HONORS REPORT

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PREDICTION AND CONTROL OF DYNAMICAL SYSTEMS: APPLICATIONS IN
COMBUSTION AND CHEMICAL REACTORS

Principal Investigator: Kenneth Showalter

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Office of Sponsored Programs

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Date Submitted: March 18, 2002

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Combustion and Chemical Reactors
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FINAL Report - Part I

- a. Submitted Papers to Refereed Journals (not yet published): 2
- b. Published Papers in Refereed Journals: 12
1. J. H. Merkin, A. J. Poole, S. K. Scott, J. Masere, and K. Showalter, "Competitive Autocatalysis in Reaction-Diffusion Systems: Exclusive Product Selectivity," *Faraday Transactions, Roy. Chem. Soc.* **94**, 53-58 (1998).
 2. S. Kádár, J. Wang, and K. Showalter, "Noise Supported Traveling Waves in Subexcitable Media," *Nature* **391**, 770-772 (1998).
 3. P. Jung, A. Cornell-Bell, F. Moss, S. Kádár, J. Wang, and K. Showalter, "Noise Sustained Waves in Subexcitable Media: From Chemical Waves to Brain Waves," *Chaos* **8**, 567-575 (1998).
 4. T. Amemiya, P. Kettunen, S. Kádár, T. Yamaguchi, and K. Showalter, "Formation and Evolution of Scroll Waves in Photosensitive Excitable Media," *Chaos* **8**, 872-878 (1998).
 5. J. Wang, S. Kádár, P. Jung, and K. Showalter, "Noise Driven Avalanche Behavior in Subexcitable Media," *Phys. Rev. Lett.* **82**, 855-888 (1999).
 6. E. Mihaliuk, H. Skødt, F. Hynne, P. G. Sørensen, and K. Showalter, "Normal Modes for Chemical Reactions from Time Series Analysis," *J. Phys. Chem.* **103**, 8246-8251 (1999).
 7. H. Sun, S. K. Scott, and K. Showalter, "Uncertain Destination Dynamics," *Phys. Rev. E* **60**, 3876-3880 (1999).
 8. P. Jung, J. Wang, R. Wackerbauer, and K. Showalter, "Coherent Structure Analysis of Spatiotemporal Chaos," *Phys. Rev. E* **61**, 2095-2098 (2000).
 9. R. Wackerbauer, H. Sun, and K. Showalter, "Self-Segregation of Competitive Chaotic Populations," *Phys. Rev. Lett.* **84**, 5018-5021 (2000).
 10. I. Sendiña-Nadal, E. Mihaliuk, J. Wang, V. Pérez-Muñuzuri, and K. Showalter, "Wave Propagation in Subexcitable Media with Periodically Modulated Excitability," *Phys. Rev. Lett.* **86**, 1646-1649 (2001).

11. E. Mihaliuk, R. Wackerbauer, and K. Showalter, "Topographic Organization of Hebbian Neural Connections by Synchronous Wave Activity," *Chaos*, **11**, 287-292 (2001).
 12. M. Hildebrand, H. Skødt, and K. Showalter, "Spatial Symmetry Breaking in the Belousov-Zhabotinsky Reaction with Light-Induced Communication," *Phys. Rev. Lett.* **87**, 883031-4 (2001).
- c. Submitted Book Chapters (not yet published): 0
- d. Published Book Chapters: 2
1. T. Amemiya, P. Kettunen, S. Kádár, T. Yamaguchi, and K. Showalter, "Perturbation-Induced Scroll Waves in Photosensitive Excitable Media," in *Proceedings of the 4th Experimental Chaos Conference*, edited by W. L. Ditto, L. Pecora, M. Shlesinger, M. Spano, and S. Vohra (World Scientific, Singapore, 1998), pp. 19-24.
 2. K. Showalter, "Controlling Chaos in Dynamical Systems," in *Self-Organized Biological Dynamics and Nonlinear Control*, edited by J. Walleczek (Cambridge University Press, Cambridge, 2000), pp. 328-340.
- e. Printed Non-refereed Technical Reports: 0
- f. Patents Filed: 0
- g. Patents Granted: 0
- h. Invited Presentations: 35
1. "Linear and Nonlinear Prediction, Filtering and Control of Dynamical Systems," Department of Physics, Technical University of Denmark; Lyngby, Denmark; April 1, 1998.
 2. "Perturbed Excitable Media," Institut für Experimentelle Physik, Otto-von-Guericke-Universität; Magdeburg, Germany; April 23, 1998.
 3. "Noise Supported Traveling Waves and Perturbation Induced Scroll Waves in Excitable Media," Complex Systems Group, Fritz-Haber-Institut der Max-Planck-Gesellschaft; Berlin, Germany; April 24, 1998.

4. "Wave Induced Chaos and Perturbation Induced Scroll Waves," Workshop on Oscillations and Spatial Structures in Chemical Systems, Department of Chemistry, H.C. Ørsted Institute, University of Copenhagen; Copenhagen, Denmark; May 7, 1998.
5. "Chemical Waves and Patterns," Department of Chemical Engineering, Prague Institute of Chemical Technology; Prague, Czech Republic; May 15, 1998.
6. "Noise Supported Traveling Waves in Subexcitable Media," Gordon Research Conference on Theoretical Biology and Biomathematics; Tilton, New Hampshire; June 7-11, 1998.
7. "Perturbed Excitable Media," Conference on Information-Based Interventions in Biological Systems, Fetzer Institute; Kalamazoo, Michigan; August 23-26, 1998.
8. "Chemical Waves and Patterns," Department of Physics, Georgia Tech; Atlanta, Georgia; November 4, 1998.
9. "The Effects of Noise in Excitable Chemical and Neuronal Systems," Swedish Medical Center; Seattle, Washington; November 20, 1998.
10. "Chemical Waves and Patterns," Department of Biology, McGill University; Montreal, Canada; December 3, 1998.
11. "Noise Mediated Wave Behavior in Subexcitable Media," Dynamics Days '99, Georgia Tech; Atlanta, Georgia; January 7, 1999.
12. "Noise Mediated Wave Behavior in Subexcitable Media," Department of Chemistry, University of Toronto; Toronto, Canada; January 19, 1999.
13. "Chemical Waves and Patterns," Department of Chemistry, Cornell University; Ithaca, New York; February 18, 1999.
14. "Dynamics and Statistics of Two Types of Spatiotemporal Chaos," Frontiers in Nonlinear Dynamics and Neurodynamics, School of Physics, Georgia Institute of Technology; Atlanta, Georgia; March 19-20, 1999.
15. "Noise Supported Traveling Waves in Subexcitable Media," Symposium on Glial-Cells, Brain Waves and Neurons: A New Perspective in Brain Research, National Annual March Meeting of the American Physical Society; Atlanta, Georgia; March 20-26, 1999.

16. "Chemical Waves and Patterns," Chaos and Complexity Center, U.S. Naval Academy; Annapolis, Maryland; March 30, 1999.
17. "Prediction, Filtering, and Control of Chemical Systems," Symposium on Control and Embedding, Fifth SIAM Conference on Applications of Dynamical Systems; Snowbird, Utah; May 22-26, 1999.
18. "Noise Mediated Wave Behavior," Gordon Research Conference on Oscillations and Dynamic Instabilities in Chemical Systems, Il Ciocco Conference Center; Barga, Italy; June 6-11, 1999.
19. "Noise Initiated and Mediated Waves in Subexcitable Media," Institut für Theoretische Physik, Technische Universität Berlin; Berlin, Germany; July 16, 1999.
20. "Noise Initiated and Mediated Waves in Subexcitable Media," Institut für Physik, Universität Potsdam; Potsdam, Germany; July 28, 1999.
21. "Noise Driven Avalanche Behavior in Subexcitable Media," Symposium on Chemical Waves, Fronts, and Patterns, National Meeting of the American Chemical Society; New Orleans, Louisiana; August 22-26, 1999.
22. "Noise Driven Avalanche Behavior in Subexcitable Media." Chemistry Department Colloquium, National Institute of Materials and Chemical Research; Tsukuba, Japan; November 22, 1999.
23. "Noise Driven Avalanche Behavior in Subexcitable Media." Kyoto Symposium on Nonlinear Science, University of Kyoto; Kyoto, Japan; November 26, 1999.
24. "Coherent Structure Analysis of Spatiotemporal Dynamics." International Symposium on Nonlinear Phenomena in Chemical Systems, Kyoto Institute of Technology; Kyoto, Japan; November 29, 1999.
25. "Stabilizing Unstable Dynamical States in Chemical Systems." Physical Chemistry Seminar, Department of Chemistry, Florida State University; Tallahassee, Florida; February 10, 2000.
26. "Chemical Waves and Patterns." Departmental Seminar, Department of Chemistry, Florida State University; Tallahassee, Florida; February 11, 2000.
27. "Chemical Waves and Patterns." Departmental Seminar, Krasnow Institute for Advanced Study, George Mason University; Fairfax, Virginia; March 3, 2000.

28. "Perturbed Excitable Media." Conference on Engineering of Chemical Complexity, Fritz-Haber-Institut der Max-Planck-Gesellschaft; Berlin, Germany; June, 14, 2000.
29. "Nonlinear Identification, Filtering and Control of Chemical Systems." Summer School on Space Time Chaos: Characterization, Control, and Synchronization; Pamplona, Spain; June 23, 2000.
30. "Chemical Waves and Patterns." Summer School on Space Time Chaos: Characterization, Control, and Synchronization; Pamplona, Spain; June 23, 2000.
31. "Self-Segregation of Competitive Chaotic Populations." Conference on Structure Formation in Chemistry and Physics; Friedrichsbrunn (Ostharz), Germany; September 28, 2000.
32. "Linear and Nonlinear Control for Chemical Systems." Departmental Seminar, Institut für Experimentelle Physik, Otto-von-Guericke-Universität; Magdeburg, Germany; October 24, 2000.
33. "Chemical Waves and Patterns." Annual Meeting of the Sonderforschungsbereich Komplexe Nichtlineare Prozesse, Fritz-Haber-Institut der Max-Planck-Gesellschaft; Berlin, Germany; November 3, 2000.
34. "Linear and Nonlinear Control for Chemical Systems." Institut für Theoretische Physik, Technische Universität Berlin; Berlin, Germany; December 7, 2000.
35. "Chemical Waves and Patterns." Gesellschaft Deutscher Chemiker, Institut für Physikalische Chemie; Wuerzburg, Germany; December 8, 2000.

i. Submitted Presentations: 0

j. Honors/Awards/Prizes:

1. Associate Editor, CHAOS: An Interdisciplinary Journal of Nonlinear Science, American Institute of Physics, 1996 - .
2. Member, Editorial Advisory Board, International Journal of Bifurcation and Chaos, 1999 - .
3. Alexander von Humboldt Senior Scientist Award, 1999.
4. Member, Editorial Advisory Board, Journal of Physical Chemistry, 2000 - .

5. Co-Chair, Gordon Research Conference on Nonlinear Science, 2001.
- k. Full-time equivalent Graduate Students and Post-Doctoral Associates: 6
 - Graduate Students: 4
 - Post-Doctoral Associates: 2
 - Female Graduate Students: 2
 - Female Post-Doctoral Associates: 0
 - Minority* Graduate Students: 1
 - Minority* Post-Doctoral Associates: 0
 - Asian Graduate Students: 2
 - Asian Post-Doctoral Associates: 1
- l. Other Funding
 1. Petroleum Research Fund, "Perturbed Excitable Media," current year funding: \$0, total funding: \$60,000, grant period: July 1998 - August 2001. This project involved studies of excitable media under the influence of external forcing and global feedback.
 2. National Science Foundation, "Spatiotemporal Dynamics in Chemical Systems," current year funding: \$110,000, total funding: \$341,589, grant period: April 1999 - March 2002. This project involves studies of inhomogeneous excitable media, pattern formation, and applications of control theory to excitable media.

FINAL Report - Part II

- a. Principal Investigator: Kenneth Showalter
- b. Phone Number: (304) 293-3435 x6428
- c. Cognizant ONR Program Officer: Michael Shlesinger
- d. Program objective: The development and application of linear and nonlinear methods for controlling dynamical systems.

- e. Significant results:

In Ref. 1 (see Part I, b.), the behavior of a system comprised of two competitive autocatalytic processes, $A + B \rightarrow 2B$ and $A + C \rightarrow 2C$, is considered. In a well-stirred batch reactor, the final equilibrium composition corresponds to a mixture of the two product species B and C, with their respective equilibrium concentrations depending on the ratio of the rate coefficients and the initial concentrations. If the same reactions are carried out in an unstirred distributed system, with local initiation of the reaction at one end of the reactor, competing propagating fronts develop. This system exhibits exclusive product selectivity, with only one of the products being formed in the reaction, provided that either the rate coefficient ratio (k_1/k_2) or the diffusion coefficient ratio (D_B/D_C) differs sufficiently from unity.

The detection of weak signals of nonlinear dynamical systems in noisy environments may be enhanced by the noise as a result of stochastic resonance (SR). In Ref. 2, we describe the influence of noise on wave propagation in the photosensitive BZ reaction. The chemical medium, which is subexcitable and unable to support sustained wave propagation, is illuminated with light that is spatially partitioned into an array of cells in which the intensity is randomly varied. Wave propagation is enhanced with increasing noise level and sustained propagation is exhibited at an optimal level, above which only fragmented waves are observed. Our study was described in a number of reports: F. Moss, "Noisy Waves," *Nature* **391**, 743-744 (1998); S. Borman, "On Wings of Noise," *Chemical and Engineering News*, February 23, 1998, p. 53; I. Peterson, "Added Noise Keeps Waves Going," *Science News* **153**(8), 113 (1998); F. E. Boas, "Useful Noise," *Harvard Science Review*, Fall 1998, p. 4.

In Ref. 3, we consider the effects of imposed noise on chemical and biological systems and offer an analysis of these effects in terms of a minimal model for excitable media. Fluctuations are important close to the threshold of pattern formation and, in fact, may dominate the spatiotemporal behavior, particularly the geometric features of large scale patterns. Well below the threshold of pattern formation, noise can sustain locally coherent patterns, which exhibit spatiotemporal fragmentation statistics described by power law relations.

Experimental and computational studies of the formation and evolution of scroll waves in three-dimensional excitable media are presented in Ref. 4. Scroll waves are initiated in the photosensitive BZ reaction by perturbing parent waves transverse to their direction of propagation. This system allows the generation of precisely oriented scroll rings by perturbing circular parent waves, permitting the study of their evolution in light-induced excitability gradients of varying intensity and direction. We find that scroll rings expand or contract depending on the strength of the imposed excitability gradient.

The interaction of noise with a subexcitable chemical system gives rise to spatiotemporal behavior with novel statistical properties. Wave behavior in a photosensitive BZ reaction, with noise imposed by a computer controlled video projector, is monitored and statistically analyzed in Ref. 5. Waves are initiated at sites where the accumulation of subthreshold perturbations induces local excitations, and waves propagate through the medium by a facilitated percolation process. We find power-law relations in the noisy BZ system that are characteristic of avalanche behavior and that suggest there are no inherent length and time scales in the system.

We present a new approach for characterizing mechanisms of complex chemical systems in Ref. 6. The determination of chemical reaction mechanisms is often difficult, particularly for complex reactions, because no systematic methods exist for identifying the essential component steps of a reaction. Recent studies have focused on the Jacobian matrix of the nonequilibrium stationary state to provide insights into the possible restrictions of any scheme of mechanistic steps. The elements of the Jacobian matrix tell how each dynamical species responds to all of the other dynamical species, as well as to itself, and therefore provides vital information on allowed and forbidden steps in a chemical mechanism. In our study, we offer a method for determining the Jacobian matrix from experimental data. Our approach is based on classical linear control theory,

where a system in a stationary or periodic state is subjected to small, random perturbations to determine the "normal modes" of the reaction. The method is demonstrated with time series from a model system, and its performance in the presence of noise is examined.

The evolution of certain dynamical systems, such as those with riddled basins of attraction, may exhibit a complex and uncertain dependence on the initial conditions. In Ref. 7, we investigate a different scenario, one where the initial conditions determine which asymptotic state is selected from an infinite number of possibilities. The phase space of such systems is foliated with "attractors," each of which is associated with a particular set of initial conditions. The associated uncertain destination dynamics can be analyzed by an appropriate reduction of the full system to a subsystem that explicitly yields the dynamics. Finally, we present a physical system, adapted from that advanced by Sommerer and Ott, to illustrate uncertain destination dynamics.

Low-dimensional chaos is now well understood and measures for its characterization are highly developed; however, the characterization of spatiotemporal chaos remains an important challenge. In Ref. 8, we describe a method for characterizing spatiotemporal dynamics that is based on a *statistical* analysis of the associated spatiotemporal behavior. We create a decomposition of the space-time matrix in terms of clusters of correlated events in space and time. The birth and death of a space-time cluster are directly related to particular dynamical events, and the cluster is therefore linked to the physical mechanism underlying the spatiotemporal behavior. Furthermore, coherent cluster decomposition allows the reconstruction of specific features of the spatiotemporal dynamics, such as cluster-size statistics and associated scaling laws. We have applied this method to a cellular excitable medium and a reaction-diffusion model describing the oxidation of CO on Pt(100). We find power-law scaling of the cluster size distribution in each model for the state of spiral turbulence as well as an increase in spatiotemporal entropy at the onset of this behavior. The key feature of this description is the decomposition of spatiotemporal dynamics into space-time clusters of coherent wave activity.

Pattern formation in competitive environments has been the subject of numerous studies in chemistry, ecology, sociology, and genetics. A class of systems, in which two populations compete for a common sustaining resource, has yielded the ecologically motivated and controversially discussed "competitive exclusion principle," where two species with similar characteristics are

unable to coexist. In Ref. 9, we present a reaction-diffusion system with chaotic dynamics that exhibits complex interface patterns arising from self-segregation behavior. We study the evolution of coupled reactions, each governed by cubic autocatalysis, which compete for a common resource. Self-segregating domains of uncorrelated chaotic populations, separated by interfaces that exhibit irregular motions on long time scales, spontaneously arise in one-dimensional configurations with random initial conditions. The self-segregation behavior found in this study is relevant to systems comprised of species with similar characteristics, and we have focused on the case of identical diffusivities and growth rates of autocatalysis. Examples of such systems include competing populations in biological ecologies as well as isomers or isotopically labeled species in competing chemical reactions.

Spatially extended dynamical systems display interesting and sometimes unexpected behavior in response to external perturbations. Temporal perturbations of excitable media, as well as spatial modulations and spatiotemporal fluctuations, give rise to new types of dynamical behavior. In Ref. 10, we study the effects of spatially homogeneous, periodic modulations of excitability on wave propagation in a subexcitable medium. Wave propagation in a photosensitive, subexcitable Belousov-Zhabotinsky medium is made possible by periodic modulation of a homogeneous illumination field. The propagation can be understood in terms of an interplay between the radial expansion of the wave and the motion of its free ends as the excitability varies periodically. This description leads to a simple kinematic analysis that provides insights into the initial conditions and forcing parameters giving rise to sustained wave propagation.

Topographically organized patterns of neural connections in which neighboring neurons project to neighboring sites in the target occur throughout the nervous system. In the vertebrate visual system, the retina sends images to be further processed in the lateral geniculate nucleus (LGN). The required topographically precise connection network develops by processes that are not fully understood, but are believed to involve electrical activity in the retina before the onset of vision. In Ref. 11, we study the evolution of initially random unidirectional connections between two excitable layers of FitzHugh-Nagumo neurons with simulated spontaneous activity in the input layer. We find in this simple model system of two coupled neural layers with initially imperfect interlayer connections a rapid topographic reorganization, arising from synchronous wave activity due to lateral

diffusive coupling within the layers and from Hebbian learning in the coupling between the layers.

In Ref. 12, we study the photosensitive BZ reaction with nonlocal coupling over a wide range of length scales, from much larger than the characteristic reaction-diffusion length scale to length scales that are comparable. The kernel of the feedback alternates from positive (activatory) for short distances to negative (inhibitory) for larger distances. We show below that such a feedback gives rise to a "Turing-like" instability, and, as a result, patterns with more than one characteristic length scale are formed.

REPORT DOCUMENTATION PAGE

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14. ABSTRACT Chemical model systems were studied to develop insights into the behavior and control of spatiotemporal dynamical systems. Noise supported wave propagation has been characterized as well as power-law relations that are characteristic of avalanche behavior. Studies were also carried out of periodically driven excitable media, spatial symmetry breaking, and the evolution of three-dimensional scroll waves. Theoretical studies were carried out on exclusive product selectivity and self-segregation in systems with competitive autocatalysis as well as coherent structure analysis of spatiotemporal chaos. Topographic organization of Hebbian neural connections, uncertain destination dynamics in coupled Lorenz systems, and normal modes for chemical reactions from time series analysis were also studied.					
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