

Modeling, Inverse Problems and Feedback Control
for Distributed Dynamical Systems

FINAL TECHNICAL REPORT
for the period

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| 13. ABSTRACT (Maximum 200 Words) Progress is reported on modeling of toxic pathways for dioxin and trichloroethylene, reduced order modeling in nonlinear coupled fluid/acoustics problems, electromagnetic interrogation of dispersive media and modeling of nonlinear hysteresis in materials. | | | | | |
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Objectives

We pursued investigations in several distinct but related areas of research. The first topic of our research involves development of models and computational packages for systems arising in nonlinear acoustics. Problems in nonlinear structural acoustics (with direct reference to AF and DoD interests) are investigated. Specifically, computational modeling of payload cavities and shear layer flow induced acoustic fields in shallow cavities such as weapon and instrument bays on military aircraft.

A second area of our research efforts entailed continuation of health sciences investigations in collaboration with scientists in the Mathematical Products Division, Air Force Research Labs, Brooks AFB. Specific topics being investigated include modeling of microwave pulses in dispersive media and their potential for use in medical imaging as well as military surveillance and detection as well as modeling of toxin distribution, metabolism and elimination in human tissues.

Status of Effort

Investigators supported under this grant have made significant progress in the following areas: (1) PBPK modeling of the toxins TCDD and TCE, (2) computational methods for control design in open cavity acoustics problems, (3) the modeling and estimation of dielectric parameters and geometry in materials using electromagnetic pulses and eddy current techniques, (4) modeling, estimation and control of smart material devices. In all cases, the basic physics or biology underlying the process is incorporated in the model and utilized to the extent possible in parameter estimation and/or control design.

Accomplishments

1. *Modeling of Toxins in Human Uptake, Metabolism and Elimination*

1a. *Hepatic Uptake and Elimination of 2,3,7,8 - Tetrachlorodibenzo-p-dioxin*

The objective of our research was the development of advanced pharmacokinetic modeling techniques to describe the transport of solutes within the liver. Our particular interest is the chemical compound 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). TCDD enters in the environment through combustion sources such as the burning of municipal and hospital wastes and in the production of certain herbicides. In particular, TCDD is an unwanted by-product in the manufacture of 2,4,5-trichlorophenoxyacetic acid (2,4,5-T) which was a primary component of Agent Orange used by US forces during the Vietnam conflict. A number of studies have been conducted to determine possible adverse health effects in Vietnam-era veterans who may have been exposed to Agent Orange. Of particular concern to researchers is TCDD's ability to produce a wide range of effects in animals following exposure, including certain types of cancer.

Physiologically-based pharmacokinetic models which have attempted to describe the hepatic uptake, distribution, and elimination of TCDD have generally used the well-stirred or venous-equilibrium model to describe events occurring in the liver. The basic assumption of this model, that the concentration of solute is uniform throughout the length of the liver acinus, does not describe the elimination of solutes with decreasing concentration gradients along the acinus following a bolus input. In addition, the "well-stirred" model cannot accommodate spatial variations in other parameters, such as enzyme activity and hepatic cell permeability.

We have developed a convection-dispersion model for the hepatic uptake and elimination of TCDD. This model incorporates the complex architecture and physiology of the human liver and includes the dynamics of TCDD interaction with two intracellular proteins, the Ah receptor and cytochrome P450 1A2 [6]. The resultant mathematical model is a nonlinear coupled system of partial differential equations and ordinary differential equations with time delay. We have established the well-posedness of the model [7], have developed approximation methodologies (with convergence arguments) for numerical simulation and the inverse problem, and are continuing initial promising simulation findings. A summary of theoretical and numerical results to date is given in the Ph.D. thesis of Musante [8] and subsequent computational results are found in [21].

1b. *Modeling of Trichloroethylene in Adipose Tissue*

In subsequent work [55] we studied three physiologically based pharmacokinetic (PBPK) models for the systemic transport of trichloroethylene (TCE), with a focus on the adipose, or fat tissue. TCE is a widespread environmental contaminant, and has been shown to produce toxic effects in both animals and humans. A key characteristic of TCE is its tendency to accumulate in fat tissue, which has a major impact on the overall systemic disposition of TCE.

We used PBPK models to predict the kinetics of TCE through the various tissues and organs, including the adipose tissue. The first model utilizes the standard "perfusion-limited" compartmental model for the fat

tissue, while the second model uses a “diffusion-limited” model to describe the transport through the adipose tissue. Both of these ODE models are based on “well-mixed” and rapid equilibrium assumptions, and do not take into account the specific and largely heterogeneous physiology of adipose tissue.

The third model we investigate is a PBPK hybrid model with an axial-dispersion type model for the adipose tissue similar to that used in the hepatic TCDD models described above. This PDE-based model is designed to capture key physiological heterogeneities of fat tissue, including widely varying fat cell sizes, lipid distribution, and blood flow properties. Model simulations demonstrate that this model may be well-suited to predict the experimental behavior of TCE in adipose tissue using parameter estimation techniques.

2. Reduced Order Modeling in Control of Open Cavity Acoustics

Aircraft with internal carriage of weapons or surveillance systems require active control strategies to limit high amplitude open bay acoustic resonances and to facilitate optimization of structure requirements and weapon/surveillance reliability. We have carried out investigations of the use of numerical simulation combined with Proper Orthogonal Decomposition (POD) model reduction methods to optimize an active control system for aircraft open cavity applications. Issues addressed include characterizing shear layer and wake resonant responses, optimal steady blowing rates, the effect of open loop harmonic perturbations, use of POD for post-processing data to reduce storage requirements, and the use of the Nelder-Mead optimization procedure. Comparison of the wake and shear layer responses reveals why a wake response in aircraft is undesirable. This study has focused primarily on a freestream flow at $M=0.85$ with a cavity of aspect ratio $l/d=4.5$. The results include the use of steady blowing injection up to $M = 0.9$ and harmonic forcing perturbations ranging in amplitude from $M=0.005$ to $M=0.45$. In the parameter space examined, fluid displacement had the largest effect. The best observed forcing reduced the buffet loading metrics by approximately 17 db. These findings are reported in [44, 48].

3. Electromagnetic Interrogation of Dielectric Materials

Significant progress has been achieved in two areas of focus in our continuing efforts on use of electromagnetic signals to interrogate materials. In collaborative efforts with the group led by Dr. R.A. Albanese, AFRL, Brooks AFB, we have developed computational methods for the inverse problems of using both conductive interfaces and acoustic wavefronts as reflectors to promote microwave pulse interrogation of materials for both dielectric properties and geometry. The details of the initial work appeared in a monograph [46] published by SIAM and in [36]. Continuing efforts involve tracking traveling acoustic waves through heterogeneous media via electromagnetic pulse reflections as well as model development for polarization in nonlinear materials.

A second focus of our efforts involves the use of ECT (eddy current techniques) to detect subsurface damage (cracks, disbonds, etc.) in structures. Eddy currents are produced in the structure under interrogation and observations of the associated magnetic fields with GMR (Giant Magneto Resistive) sensors can be used to detect structural anomalies. We have successfully developed reduced order computational methods (reported in [33, 34, 35]) based on Karhunen - Loève reduced basis techniques for the associated inverse problems. This is a joint effort with a NASA team of scientists led by Dr. W. Winfree (NASA Langley Research Center) but it has great relevance to AF and DoD needs in the area of damage detection in aircraft and other military structures. We have demonstrated the ability to determine both geometry and depth of subsurface occlusions. These techniques have recently been successfully validated in experimental efforts at NASA Langley.

4. Model Development and Control Design for Smart Materials with Hysteresis

We have significant progress on modeling and design of smart material devices with focus in several distinct but related areas.

In collaborations with scientific teams at Lord Corporation, we have made major advances in two types of smart material vibration suppression type devices. Significant progress has been made in understanding the constitutive relationship between applied magnetic field and rheological response in magnetorheological (MR) fluids. Computational methods (resulting in software packages now being used at Lord in material design) based on both homogenization and fast multi-pole methods (for complete near field particle force interactions) have been successfully developed and experimentally validated [20, 24, 32, 43]. A second project with Lord scientists deals with the understanding of nonlinear hysteresis in elastomers (filled viscoelastic rubber-like materials structures used in damping devices). Our contributions [31, 37, 51, 52] have involved leading edge technology and the models have been experimentally validated for structural samples in both shear and extension. Recent extensions and transitions have resulted in a Rubber Division, American Chemical Society

best paper award for the paper [53]. The computational ideas developed in this context have proved useful in our investigation on characterization of shear waves in viscoelastic materials [50] as well as modeling of polarization in nonlinear materials.

A second area of investigation has focused on the development of models, commensurate numerical and parameter estimation methods, and model-based control techniques for high performance smart material transducers which exhibit hysteresis and constitutive nonlinearities. The initial emphasis centered on the ferromagnetic material Terfenol-D and the ferroelectric compounds PZT and PMN due to their prevalence in broadband applications. The scope of the investigation has recently been expanded to include certain ferroelastic compounds, including the shape memory alloy Nitinol, due to their capability for generating large strains. The commonality between these compounds is provided by the domain structure inherent to the materials, and one goal of the investigation is to utilize this ferroic structure to develop unified low-order models which facilitate subsequent control design. The consideration of model development and control design as symbiotic processes provides the possibility for significantly expanding the capability of high performance smart material transducers in aeronautic, aerospace, defense, and industrial applications.

Models and control algorithms were first developed for magnetostrictive transducers employed in applications which require large input forces (e.g., sonar transducers, high speed milling lathes). The initial models focused on the quantification of the direct and converse magnetoelastic effects [10, 57, 60, 61, 62, 63] while later components of the investigation have centered on the incorporation of frequency and design properties of the transducers [64, 66]. Both theoretical and implementational issues concerning the design of control algorithms which utilize the models have also been investigated in the context of magnetostrictive transducers [68, 69, 77, 78]. As reported in [69], the use of inverse compensators constructed from the nonlinear hysteresis models have yielded accuracies of ± 2 microns at a rotation rate of 3000 rpm for a milling machine employing a magnetostrictive transducer.

A second facet of the investigation has focused on the development of analogous models for ferroelectric materials including the electrostrictive compound PMN and piezoceramic actuators/sensors (PZT). The initial theory for ferroelectric materials was presented in [65, 70, 71] and extensions to incorporate the temperature-dependence in relaxor ferroelectric materials is summarized in [72]. The extension of the models to piezoceramic transducers was reported in [73, 74, 75, 76]. Finally, results from an initial investigation incorporating the model-based compensators into amplifier design are reported in [58, 59]. The extension of the control techniques described in [69, 77, 78] to piezoceramic and electrostrictive actuators is under current investigation.

A summary of the common issues being addressed in the development of models, numerical algorithms and control techniques for high performance transducers which utilize these materials is provided in the chapter [67]. This reference also indicates some of the issues associated with the extension of these techniques to shape memory alloys which is also under current investigation.

Personnel Supported

H.T. Banks, R.C. Smith, A.B. Cain, D. Rubio, G.A. Pinter, R.C.H. del Rosario, D.M. Bortz, L.K. Potter, J.K. Raye, S.C. Beeler and B. Browning.

Interactions

H.T. Banks - Presentations

1. ARO Damping Workshop, VPISU, Blacksburg, VA, October 19-22, 1998.
2. Intl. Conf. on Semigroups of Operators: Theory and Applications, Newport Beach, Ca, December 14-18, 1998.
3. Institute for Mathematical Systems, Universitat Groningen, The Netherlands, January 6-9, 1999.
4. SPIE Symposium on Smart Structures and Materials, Newport Beach, CA, March 1-4, 1999.
5. AMS Western Regional Conference, Las Vegas, NV, May 9-11, 1999.
6. AIAA/CEAS Aeroacoustics Conference, Bellvue, WA, May 10-12, 1999.
7. NSF Workshop on Active Flow Control, University of California, San Diego, May 31-June 1, 1999.
8. SIAM Math-In-Industry Workshop, Harvey Mudd College, Claremont, CA, June 16-19, 1999.
9. Workshop on Control, System Theory and Mathematical Modeling, Gadjah Mada University, Yogyakarta, Indonesia, July 19-23, 1999.

10. International Conference on Math and Its Application, SE Asian Math Society, Gadjah Mada University, Yogyakarta, Indonesia, July 26-29, 1999.
11. Intl. Workshop on Systems with Hysteresis, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, September 20-24, 1999.
12. SIAM Conf. in Industrial Applied Mathematics, Raleigh, NC, Oct. 10-12, 1999.
13. Conf. on Advances in Control of Nonlinear Distributed Parameter Systems, Texas A&M University, College Station, TX, Oct. 22-23, 1999.
14. Invited Survey Lecture, SPIE Symposium on Smart Materials and Structures, Newport Beach, CA, March 5-9, 2000.
15. Trends in Dynamical Systems, Institute of Mathematics, Universität Graz, Graz, Austria, March 16-18, 2000.
16. Plenary Lecture, SIAM-SEAS Annual Conference, Univ.-Georgia, Athens, GA, March 24-25, 2000.
17. AMS Symposium on Mathematical Models in the Biological and Physical Sciences, Univ. Louisiana-Lafayette, April 14-16, 2000.
18. Workshop on Principal Orthogonal Decomposition and its Applications, Graz, Austria, May 25-27, 2000.
19. Conference on Optimal Control of Complex Dynamical Structure, Mathematisches Forschungsinstitut Oberwolfach, Germany, June 4-10, 2000.
20. Plenary Lecture, 2nd European Conference on Structural Control, Ecole Nationale des Points et Chaussées, Champs-sur-Marne, France, July 3-6, 2000.
21. Conference on Computation and Control VII, Bozeman, MT, August 1-4, 2000.
22. International Workshop on Hysteresis, Univ. Ill.-Chicago, August 28-30, 2000.

R.C. Smith - Presentations

1. SPIE's Sixth Annual Symposium on Smart Structures and Materials, Newport Beach, CA, March 1-4, 1999.
2. Eighteenth Annual Conference on Properties and Applications of Magnetic Materials, Illinois Institute of Technology, Chicago, IL, April 28, 1999.
3. 1999 U.S. Navy Workshop on Acoustic Transduction Materials and Devices, Penn State University, State College, PA, April 14, 1999.
4. Colloquium, Department of Mathematics, Virginia Polytechnic Institute and State University, Blacksburg, VA, October 23, 1998.
5. Colloquium, Department of Applied Mechanics and Engineering Sciences, University of California, San Diego, CA, March 5, 1999.
6. Colloquium, Department of Electrical Engineering and Institute for Systems Research, University of Maryland, College Park, MD, March 15, 1999.
7. "Modeling and Control Issues Concerning Smart Materials with Hysteresis," NSF-CBMS Workshop on Control of Distributed Parameter Systems, University of Nebraska, Lincoln NE, August 10, 1999.
8. "Modeling and Control Issues Concerning Smart Materials with Hysteresis," Fourth ARO Workshop on Smart Structures, Penn State University, State College, PA, August 16, 1999.
9. "Modeling and Control Issues Concerning Smart Materials with Hysteresis," Colloquium, Bradley Department of Electrical and Computer Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, September 20, 1999.
10. "Modeling and Control Issues Concerning Smart Materials," Session on Engineering Acoustics: Transducer Loss Mechanisms, 138th Meeting of the Acoustical Society of America, Columbus, OH, November 1, 1999.
11. "Modeling and Control Issues Concerning Smart Materials with Hysteresis," Adaptive Structures and Material Systems Symposium, 1999 ASME International Mechanical Engineering Congress and Exposition, Nashville, TN, November 17, 1999.
12. "Modeling Aspects Concerning THUNDER Actuators," Adaptive Structures and Material Systems Symposium, 1999 ASME International Mechanical Engineering Congress and Exposition, Nashville, TN, November 18, 1999.

13. "Modeling and Optimization Issues Concerning a Circular Piezoelectric Actuator Design," Adaptive Structures and Material Systems Symposium, 1999 ASME International Mechanical Engineering Congress and Exposition, Nashville, TN, November 18, 1999.
14. "Modeling and Control Issues Concerning Smart Materials with Hysteresis," Smart Materials Symposium, Fall Meeting of the Materials Research Society, Boston, MA, December 2, 1999.
15. "Inverse Compensation for Hysteresis in Piezoceramic, Electrostrictive and Magnetostrictive Materials," Session on Control of Distributed Parameter Systems: New Approaches and Applications, 38th IEEE Conference on Decision and Control, Phoenix, AZ, December 9, 1999.
16. "A Domain Wall Model for Hysteresis in Piezoelectric Materials," SPIE's Seventh Annual Symposium on Smart Structures and Materials, Newport Beach, CA, March 7, 2000.
17. "Control Strategies for Smart Material Systems with Hysteresis," SPIE's Seventh Annual Symposium on Smart Structures and Materials, Newport Beach, CA, March 7, 2000.
18. "A Temperature-Dependent Constitutive Model for Relaxor Ferroelectrics," SPIE's Seventh Annual Symposium on Smart Structures and Materials, Newport Beach, CA, March 8, 2000.
19. "A Magnetoelastic Model for Magnetostrictive Sensors," 2000 U.S. Navy Workshop on Acoustic Transduction Materials and Devices, Penn State University, State College, PA, April 12, 2000.
20. "A Domain Wall Model for Hysteresis in Piezoelectric Materials," 2000 U.S. Navy Workshop on Acoustic Transduction Materials and Devices, Penn State University, State College, PA, April 13, 2000.
21. "Modeling and Control Issues Concerning Smart Materials with Hysteresis," Colloquium, Department of Electrical Engineering, Iowa State University, Ames, IA, May 12, 2000.
22. "Development and Validation of a Hysteresis Model for Piezoelectric Actuators," Session on Analytic and Experimental Characterization of Piezoelectric Materials, Third SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, May 23, 2000.
23. "Partial and Full Inverse Compensation for Hysteresis in Smart Material Systems," Session on Control of Distributed Parameter Systems, 2000 American Control Conference, Chicago, IL, June 29, 2000.

D.M. Bortz

1. AIAA Conference, Maui, June 12-14, 2000.

Transitions

1. PBPK Modeling: Development of models and associated software in conjunction with R. Albanese's group at AFRL (see below) and M. Evans, EPA (tel. 919-541-0838). These models have great relevance to AF and DoD due to the presence of TCDD and TCE at many military bases.
2. Nonlinear Acoustics: Development of models and associated software for simulations and control in shallow cavity acoustics involves collaboration and interaction with Mick Stanck, AFRL, Wright Patterson AFB.
3. Electromagnetic Interrogation of Dispersive Media: Problem formulation and method development involves close collaboration with Dr. Richard Albanese (tel: (210) 536-5710) and colleagues at AFRL, Brooks AFB. The reflection acoustic grating problems mentioned above have direct application to Albanese-led efforts on material detection and interrogation of interest to AF and DoD (location of subsurface mines, bunkers, characterization of weapons systems stealth technology). The project using eddy current techniques in subsurface damage detection is in collaboration with Dr. William Winfree (tel:(717)864-4963) and colleagues at NASA Langley Research Center, Hampton, VA. The methods developed to date are being used in experimental efforts at NASA Langley in our efforts with this group.
4. Modeling of Smart Material Damping Devices: Our efforts on inverse problem methodology have been directly transitioned to problems on design of "smart" fluids and elastomers at Lord Corporation, Cary, NC. Collaborative efforts with scientists (contact: Mark Jolly (tel:(919) 469-2500, ext. 2335)) have benefited enormously from use of computational ideas and methods developed under AFOSR support through this grant and its predecessors. The efforts on magnetostrictive transducers including models, numerical methods and control techniques has been transitioned to Etrema Products, Ames, IA, where our software is being used in design. Contact points are R. Zrostlik (tel:(515) 296-7953) and J. Slaughter (tel: (515) 296-6826).

Honors/Awards

- Banks, IEEE Fellow, 1994.
- Banks, IEEE CSS Systems Technology Award, 1996.
- Banks, Distinguished Alumnus Award, Purdue University, 1998.
- Banks, Elected Chairman, SIAM Board of Trustees, 1999; re-elected, 2000.
- Banks, Institute of Physics Fellow, 1999.
- Banks, Alumni Distinguished Graduate Professor, NCSU, 2000.
- Banks (with Yeoh and Pinter), Best Paper Award, 158th Meeting Rubber Division, American Chemical Society, Cincinnati, OH, October, 2000.
- Smith, Early Achievement Award, Iowa State University, 1997.
- Banks and Smith (with Silcox), 1995 ASME Adaptive Structures "Best Paper Award in Structural Dynamics and Control", Adaptive Structures Forum, Salt Lake City, Utah, April, 1996.

Publications

Publications of work partially supported under this grant during the reporting period are listed below as references.

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