Computational Methods for Control of Nonlinear Fluid/Structure Problems

Final Technical Report

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13. ABSTRACT *(Maximum 200 words)*
Status of efforts are reported on the following topics: (1) modeling and estimation problems associated with subsurface contaminant transport problems; (2) a conservative second-order semi-Lagrangian scheme for a tracer governed by the shallow water equations; (3) development of physiologically based pharmacokinetic models of the behavior of 2,3,7,8-TCDD in humans; (4) radio frequency bonding of adhesives in composites; and (5) identification of polarization and description of electromagnetic field energy in material, including tissue.

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Objectives

This grant was for graduate student support in research efforts which involve theoretical, computational, and experimental research in the general area of control of nonlinear fluid/structure interactions. This work, to be pursued in an integrated, multidisciplinary approach, involved basic research on the modeling, identification, and control and computation in (i) flow control, (ii) smart materials structures, (iii) control of nonlinear fluid/structure interaction models, and (iv) E and M fields in tissue.

Status of Efforts (Final)

During the grant period a number of primary graduate student investigators (under the guidance and in collaboration with faculty investigators) have pursued studies and made progress in the following areas:

I. Kendall Bailey and Mike Jeffries investigated modeling and estimation problems associated with subsurface contaminant transport problems. Motivated by experiments conducted on Columbus AFB, Mississippi, by AFAL/EQ personnel, these numerical modeling efforts have produced new methods for determining basic flow parameters, such as hydraulic conductivity, from experimental (field) data. Bailey has completed a MS and graduated. Jeffries is continuing efforts on a Ph.D.

II. Tammy Simon applied and tested a conservative second-order semi-Langrangian scheme for a tracer governed by the shallow water equations. She compared the new method with lower-order conservative methods and higher-order non-conservative methods. These comparisons demonstrate the new method has accuracy similar to other more commonly used non-conservative order methods while maintaining strict conservation. Her efforts have now evolved to work on control of magnetorheological fluids. Methods for computing the MR response to an applied magnetic field are being developed. She is making excellent progress in her Ph.D. thesis research.

III. Cindy Musante has investigated development of physiologically based pharmacokinetic models of the behavior of 2,3,7,8-TCDD in humans. In particular, a partial differential equation based model has been developed to describe the kinetic of elimination of dioxin by the liver. This model includes matabolism and binding protein in the liver and has been developed in collaboration with scientists in the Mathematical Products Division, Brooks AFB, San Antonio, TX. Cindy will spend the summer of 1997 with Dr. R. Albanese's group at Brooks AFB and is currently developing numerical simulation techniques for the model. She should complete her Ph.D. thesis in late 1997 or early 1998.

IV. Melissa Goodhart has investigated radio frequency bonding of adhesives in composites. Modeling of the nonlinear heating process involving electromagnetic heating, exothermic reaction of the adhesives and nonlinear diffusion and cooling has been investigated

with computational and experimental efforts (in collaboration with Lord Corporation). Operator splitting techniques have been developed for 3-D nonlinear heat transport. Methods are being developed to be used in modifying the online production in automotive assembly plants. A paper reporting these efforts is in preparation. This early work will be the foundation of Melissa's Ph.D. research.

V. Michael Buksas has made outstanding progress on identification of polarization and description of electromagnetic field energy in material, including tissue. Computational methods for both forward simulations and inverse problems have been developed and tested. These efforts are in close collaboration with Dr. Richard Albanese and Dr. Yun Wang, Mathematical Products Division, Brooks AFB. Recent significant efforts involve the use of E & M probes with our models to interrogate the geometry of a target.

Efforts on two of the topics above (III and V) have resulted in major results of interest to AF researchers. These will be outlined in more detail below.

A. Modeling the Hepatic Uptake and Elimination of 2,3,7,8 - Tetrachlorodibenzo -p-dioxin

The objective of this research is 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 U.S. 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 [M], [BMT]. The resultant mathematical model is

a nonlinear coupled system of partial differential equations and ordinary differential equations with time delay. We have studied the well-posedness of the model and are currently developing numerical methodologies for numerical simulation and the inverse problem.

B. Estimation of Electromagnetic Dispersion

Microwave images of tissue structures and soils play very important roles in many areas, including clinical and environmental medicine. These microwave images are useful in detection/enhanced treatment of abnormality of human organs and tissue, and detection/remediation of underground toxic wastes. The electromagnetic properties of a medium are generally characterized by its electric and magnetic polarization mechanisms and its static conductivity. Our recent efforts involve the development of partial differential equation (Maxwell's equations) based identification techniques for dispersion in physical and biological distributed parameter systems, with those for living tissue being a special case.

Our initial efforts have focused on a time domain approach for the investigation of dispersion mechanisms of a medium in electromagnetic field problems. Maxwell's equations coupled with a generalized electric polarization model are considered. The polarization is given in terms of a convolution of the electric field with an impulse response function. This model includes time hysteresis mechanisms as well as the usual ordinary differential equations (e.g. Debye, Lorentz and multiples of these) for dispersion. Existence, uniqueness and continuous dependence of solutions on data have been given for a one-dimensional (p-polarized plane waves) dispersive medium case in [BBW]. Estimation of electromagnetic properties of media have been demonstrated via numerical examples. Parameters representing the electromagnetic property of a medium may include the static permittivity, relaxation time, natural frequency, static conductivity, etc. depending on the polarization model chosen.

The methodology for estimation of electromagnetic parameters has also been used as a basis for interrogation of geometry of targets. Initial efforts based on "method of mappings" techniques used in optimal shape design offer great promise in using electromagnetic pulse probes to determine geometry as well as material dielectrics when the interrogated body has partial boundaries of supraconductive material.

References

[1] [M] C.J. Musante, "A Dispersion Model for the Hepatic Uptake and Elimination of 2,3,7,8-Tetrachlorodibenzo-p-dioxin", Annual Meeting of the Southeastern Atlantic Section of SIAM, Clemson, SC, March, 1996.

[2] [BMT] H.T. Banks, C.J. Musante, and H.T. Tran, "A Dispersion Model for the Hepatic Uptake and Elimination of 2,3,7,8-Tetrachlorodibenzo-p-dioxin," in preparation.

[3] [BBW] H.T. Banks, M.W Buksas, and Y. Wang, "A Time Domain Formulation for Identification in Electromagnetic Dispersion," CRSC TR96-30, October, 1996; J. Math. Systems, Estimation and Control, to appear.

Accomplishments and New Findings

Accomplishments include the development of substantial software packages that are being used to carry out the investigations in projects I, IV, V listed above.

Personnel Supported

M. Bailey, M. Jeffris, T. Simon, C. Musante, M. Goodhart, M. Buksas, and D. Stevens.

Publications

See references in Status Report

Interactions and Transitions

Major ongoing interactions with the Lord Corporation and several Air Force groups; see above summary of effort. See also please Final Technical Report on parent grant AFOSR-49620-93-1-0198.

New Discoveries, Patents, and Inventions

None.

Honors and Awards

M. Bailey, GAANN Fellow;
T. Simon, GAANN Fellow;
M. Goodhart, GAANN Fellow;
M. Buksas, GAANN Fellow;
C. Musante, GAANN Fellow.