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Studies in Energetic Material Dynamics

Report 1

for the period June 1, 1981 to May 30, 1982

Herschel Rabitz
Principal Investigator

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energetic materials, intramolecular energy transfer, dissociation, kinetics, sensitivity analysis, non-equilibrium processes

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This research is for the study of microscopic processes relevant to the decomposition of energetic materials. The research has three components: (a) critical parameter studies in bulk systems, (b) intramolecular energy transfer in polyatomic molecules and (c) the application of new numerical tools to decomposition kinetics.

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Studies in Energetic Material Dynamics

by Herschel Rabitz
Princeton University

1. Contract Description.

This research is for the study of phenomena relevant to the behavior of energetic materials. The storage and transfer of energy in chemical systems is of concern for a host of practical and fundamental reasons. The present research is divided into three primary categories: (a) critical parameter studies of bulk dynamical systems, (b) intramolecular energy transfer in polyatomic molecules and (c) the application of new numerical tools to decomposition kinetics. All of these studies are interrelated but each has its own definite goal. The first topic (a) aims to further develop and exploit new sensitivity analysis techniques for the determination of key molecular parameters controlling bulk kinetic phenomena. Part (b) of the research focuses on the elementary step of how energy can be redistributed within a molecule as a forerunner to chemical decomposition. Finally, part (c) will bring to bear the powerful multi-grid technique capable of solving the non-linear equations of decomposition kinetics. All aspects of the research utilize a variety of techniques, many of which will be developed under this contract.

2. Scientific Problem.

The chief unknown problem in the area of energetic material dynamics is a knowledge of what processes *are taking* place at a microscopic scale. This question involves both physical and chemical processes.

3. Progress.

Research is being carried out on three distinct but interrelated topics. A summary of these activities is given below.

a. Intramolecular Energy Transfer and Dissociation. This study concerns the dynamics of molecules especially under conditions where they contain sufficient excess internal energy for bond rupture to occur. The evolution of such molecular systems is basic to dissociative dynamics of energetic materials and more generally to all aspects of molecular kinetics. A quantum mechanical approach is being taken to this problem and the theory along with numerical calculations are underway for reactive and non-reactive processes.

b. Stochastic Kinetics and Sensitivity Analysis. This study concerns bulk kinetic phenomena which inherently contain parameters such as rate constants which are fluctional in nature. This circumstance can arise due to thermal noise or concentration fluctuations. The sensitivity and related stability analysis of stochastic kinetic equations is being investigated with an emphasis on systems capable of exhibiting unstable behavior.

c. The Coupling of Non-Equilibrium Transport and Relaxation Processes. In reacting fluids, there is concomitant mass, energy and momentum

transport processes. Such systems are inherently under non-equilibrium conditions and a basic question concerns the degree of coupling between these effects. Our present research is focusing on coupling between the non-equilibrium transfer processes and systems where there are significant mass differences between the various atomic and molecular species.

4. Publications.

a. D. Dacol and H. Rabitz, "Arbitary Order of Functional Sensitivity Densities for Reaction-Diffusion Systems", J. Chem. Phys., submitted.

b. D. Dacol, J. Tully and H. Rabitz, "The Stability of Kinetic Systems in the Presence of Internal and External Fluctuations", to be published.

c. J. Savchik and H. Rabitz, "Kinetic Relaxation of a Binary Gas Mixture in the Presence of Non-Equilibrium Temperature and Velocity Flow Fields", J. Chem. Phys., submitted.

5. No unspent funds are expected to be remaining in the contract at the end of the first year.

6. Other Research Support.

Collision studies of gaseous molecular lasers (ONR, N00014-75-C-0478), inversion of spectral line shapes to yield collisional rate constants (with J. Gelfand and R. Miles, (ONR, N00014-78-C-0721), finite element method for atom-molecule reactive scattering (with A. Cakmak, (NSF, CHE-7909409), joint experimental and theoretical investigation of collisional relaxation and chemical dynamics of highly excited molecules (with J. Gelfand and R. Miles, NSF, CHE-7116985), dynamical studies of molecular systems, DOE (EY-76-F-02-2542), combustion chemistry of vibrationally excited oxygen, ARO, (with R. Miles and J. Gelfand, DAA-G29-82-K-0046).