SHORT-TERM VISITS FOR COLLABORATIVE RESEARCH

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13. ABSTRACT (Maximum 200 words)

Two Russian scientists were invited to spend six months at North Carolina State University, Raleigh, NC, to develop and promote individual research interactions that are of mutual benefits in the field of shock compression chemistry. The principal results of their visits are (1) up-to-date reviews and evaluations not only of their own research activities, but also of Russian publications since 1986, (2) a comparative study of U.S. and Russian approaches to the modeling of heterogeneous continua, and (3) the development of a new computational technique to analyze and interpret the mesoscale response of heterogeneous media to shock loading. A further extension of the third project will be continued at one of the home institutions in Russia under the auspices of the program titled "Industrial Partnering with the New Independent States of the Former Soviet Union."

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I. Introduction

The goal of the NCSU exchange program was to explore and establish potential areas of collaborative research with leading Russian scientists in the areas of the constitutive modeling of shock compression chemistry in heterogenous powder media. Two visitors, Profs. N. Kh. Akhmadeev and S. G. Psakhie, were chosen based mostly on their publication records and the compatibility of their work to the on-going research programs at North Carolina State University.

Prof. Akhmadeev is Head of the Laboratory of Explosion and Shock Processes at the Institute of Mechanics, Russian Academy of sciences, Ufa. His publication records include 3 books, 36 journal articles, and numerous technical reports. His activities cover a wide spectrum of areas such as mechanics and physical chemistry of multiphase media, kinetic processes and shock phenomena in solids, dynamics of porous media, dislocation theory, modeling of systems with distributed parameters, and non-stationary flows in heterogeneous media.

Prof. Psakhie is Head of the Computer Simulation Department, Russian Materials Science Center (Tomsk) and Professor of Physics at the Tomsk State University, Tomsk. He has published 3 books and 62 journal articles. His research activities cover areas such as experimental and theoretical investigations of materials response under different types of loading, computer simulation, and computer aided design of new materials and technologies.

II. Summaries of Activities

A. Prof. N. Kh. Akhmadeev

Prof. Akhmadeev arrived in Raleigh, NC with his family in November of 1993 and returned to Ufa in June 1994. Initially he delivered a series of lectures on his research activities in the modeling of heterogeneous media undergoing physico-chemical transformations. The titles of these lectures were

1. Modeling of Shock-Induced Phase Transitions,
2. Modeling of Shock-Induced Solid State Chemical Reactions,

3. Modeling of Damages under Shock Loading.

His lecture notes were later compiled as a internal report [1]. A selected portion of these lectures was presented in his paper "Modeling Physical and Phsyical Transformations" at the ARO Workshop on Shock Synthesis of Materials, Georgia Institute of Technology, May 24, 26, 1994.

He then conducted a comparative study of his theory of heterogeneous media with the continuum mixture theory extensively used for explosives by M. Baer and J. Nunziato at Sandia National Laboratories. His findings show that they are similar, but there exist some fundamental differences resulting from the basic assumptions imposed on the response behavior of heterogeneous media. One such difference is the meaning of overall stress and its relation to stress in constituents. There is evidence that the choice of the continuum postulates may be critical in the interpretation of shock data involving chemical reactions in granular materials [2].

One characteristic feature of the Akhemadeev model not found in most continuum models such as the Sandia model is its explicit treatment of elastic-plastic behavior. Although the approach is phenomenological, the model is capable of describing the critical phenomena such as pore collapse in terms of plastic response of constituent materials. Therefore, an evaluation is being made of the Akhemadeev model, to see whether we can incorporate his approach to generalize our constitutive model, called VIR, for shock-induced chemical reactions in mixed powders. This model has been successfully applied to describe a variety of reactive powder mixtures. But it is a hydrodynamic, multiphase model and does not consider the plastic response of constituents explicitly. Pore collpase is treated by a standard P-α model.

Recently Prof. Akhmadeev informed us (1) that after returning to Ufa he undertook the task of integrating his work on porous solids and chemical reaction and has developed a computational model that can describe chemical reactions in two phase, porous, elastic-plastic media, and (2) that they have successfully applied this model to the experimental investigation of the Sn+S mixture by Prof. S. S. Batsanov. No detail is available at the present time.

Also, Prof. Akhmadeev conducted an in-depth review of Russian literature on shock chemisty and related subjects. His attention was focused on investigations since the publication of Batsanov's comprehensive review in 1986. His notes were collected as an internal report [3]. Initially this activity began as a joint project between Profs. Akhmadeev and Psakhie, but midway it became two separate projects.

There were no surprising findings (to this author) in both reviews in terms of materials, equipment and measurements, and theories. But, one cannot fail to be impressed at the variety of Russian activities and sustained interest in shock chemistry, and their applications to materials synthesis over a period of several decades. They also show that there is still a lack of basic, mechanistic understanding of shock-induced chemical reactions at the shock front where the conditions are most favorable for non-equilibrium processes.

B. Prof. Serguei G. Psakhie

Prof. Psakhie arrived in Raleigh in late January of 1994 and is scheduled to depart for Russia on December 18, 1994. In March he returned to Russian for three weeks for the funeral of his mother-in-law. Happily, his visit at NCSU has been extended for an additional period of six months by a support from Sandia National Laboratories to continue the joint development of a new, generalized simulation and analysis tool called Element Dynamics.

Shortly after retuning to NCSU in April, Prof. Psakhie began a series of lectures on the Element Dynamic method and a cellular automata technique for description of SHS and shock chemistry. His lecture notes were collated as an internal report [4]. Also a summary of research activities in his department was presented at the ARO Workshop on Shock Synthesis of Materials, at Georgia Institute of Technology, May 24-26, 1994.

As mentioned above, Prof. Psakhie reviewed the Russian literature on shock chemistry. His emphasis is placed on shock-loading techniques for materials synthesis and models of microscopic mechanisms under shock compression. His review, containing approximately 200 references, is published as an internal report [5].

III. Accomplishments

The most significant accomplishment that has come out of the present exchange program is the joint development of a new, generalized Discrete Element Dynamics (DED) program with Prof. Psakhie. Some promising capabilities of this program were presented at the Materials Week '94, Rosemont, Il, October 2-6, 1994. One striking example is the prediction of mass mixing in powders under high pressure shock loading. Such a calculation cannot be performed by codes that are based on continuum mechnics. Mass transport such as diffusion is handled phenomenologically.

The DED technique, originally developed for the description of materials such as rocks and sand, is an alternative approach to those based on continnum mechanics for the investigation of dynamic materials response. DED employs a system of discrete mass particles and interactions that are based on contact forces between them. The kinetics of the particles are governed by the Newtonian rigid body.

Psakhie's DED has two unique features not found in others [5]. They are (1) the multi-particle representation of a single grain and (2) a model of bonding and debonding of particles. However, the description of plastic response of granular materials was friction-like and quite inadequate for the description of plastic behavior. Also, the algorism for chemical reactions was not based on physical mechanisms, but a mathematical concept of cellular automata.

The new program is based on a physically realistic model of plasticity and chemical reactions. It has been tested for the compaction of heterogeneous powders under a variety of shock loading. The results show not only features that have been predicted by continuum based calculations, but also heterogeneous effects at the particle level.

A further development of this program including chemical reactions will be continued by Prof. Psakhie's group beginning in January 1995 for two years under the auspicies of the program "Industrial Partnering with New Independent States of the Former Soviet Union" through Sandia National Laboratories. Continuation of the effort at North Carolina State University will require new funding.

IV. Conclusion

We have successfully established and fostered indivdual research interactions with two leading Russian scientists in the area of computatioal modeling of shcok chemistry in heterogeneous media. We have developed a new computational method as well as a computer program that is capable of investigating mesoscale, heterogeneous phenomena at the particle level under a variety of loading conditions. For example this program can be used to study the mesoscale mechanisms in the shock compaction of powders, mass mixing, the formation of hot spots, spalling, effects of anisotropy in dynamic materials response, initiation of chemical reactions, bonding of particles under shock compression, and even the large deformation of polycrystalline solid materials. It can also be used for large scale phenomena such as impact penetration and structural response under dynamic loading.

V. References

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