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NARRATIVE:

Mathematical Simulation of the Fractured Subsurface Reservoir Contamination by Hazardous Reactive Chemicals

Significance

I am applying for a CSU Research Grant, which can allow me to devote more time for my research efforts in the area of mathematical modeling of groundwater contamination. The significant outcomes of the project are expected, including significant research advances in the area of ecology and environment sustainability, publication of the articles in reputable journals, involvement of undergraduate students and preparation of the proposal for the external funding.

I started preparation to this project 8 years ago, when I was employed by Tohoku University, Japan. Tohoku University was selected among the leading Japanese universities to provide a leadership in assessing the prospective sites for storage of the hazardous materials, for proposing the effective natural and engineered barriers for protecting the surrounding subsurface domains from the contamination, and for predicting the outcomes of accidental leakage of the hazardous contaminant. During that preparation period I was involved in collecting the experimental data, studied publications related to the problem, and visited several research institutions involved in waste management in Japan and also I spent 2 weeks in Lawrence Berkeley National Laboratory. During the past 7 years I developed effective mathematical methods that allow me to produce the adequate mathematical model capable to predict an outcome of the subsurface reservoir contamination with hazardous reactive chemicals. These methods are discussed in my recent book published by Tohoku University Press.

Aquifer contamination by reactive hazardous chemical elements is an actual environmental problem for all developed countries. In many countries it is common to use fractured bedrock aquifers as water supply and possible contamination of these aquifers is becoming a serious problem. The fractured porous aquifers are formed by porous rock matrixes of nonzero porosity dissected by a fractal-type network of fissures (see Fomin et al., 2005-2011 in CV section) of high hydraulic conductivity. For fractured porous medium, it can be said that fluid is stored in the porous elements and transported along the fissures. Water flow and solute transport by seeping groundwater are relatively slow, and it is not possible to carry out experiments over thousands of years and hundreds of meters of interest. Instead, one has to rely on models that describe the processes and mechanisms that would be dominant over long periods of time. It is therefore essential to understand the key processes well enough that credible predictions can be made using models based on well-established laws of nature. The difficulties in applying the basic laws of mass and momentum conservation arise mainly from the fact that the location, orientation and detailed hydraulic properties of the fractures cannot be measured in detail. This lack of measurement data makes it difficult to build models that account for all the processes. Simplifications are therefore made in an attempt to bring out the dominant processes.

Recently I suggested (Fomin et al., 2005-2011 in CV section) a relatively simple mobile/immobile model, with fractal retention times, capable of simulating the anomalous character of solute concentration distributions for the flows in heterogeneous media of fractal geometry. In the field experiments carried out by my co-authors (Fomin et al., 2006 and 2010 in CV section) for the solute transport in highly heterogeneous media, the solute concentration profiles exhibited faster-than-Fickian growth rates, skewness, and sharp leading edges. These effects cannot be predicted by the conventional mass transport equations. It was demonstrated in a number of publications of S. Fomin that fractional differential equations can simulate the anomalous character of solute transport in highly heterogeneous media. In the present study a mathematical model of the reactive contaminant transport in a single fracture (within the fractured aquifer) surrounded by the porous rocks will be derived and analyzed. Through the use of fractional derivatives, the model will account for contaminant exchange between the fracture and porous rock matrix of fractal geometry and non-local character of chemical reactions within the contaminant trapped by the porous medium. For the case of an arbitrary time-dependent source of contamination located at the inlet of the fracture, closed-form solutions for solute concentration in the fracture and in the confining rock will be obtained.

The principal targets of the proposed research are:

1. Derivation, evaluation and validation of the mathematical model of the contaminant transport in a fractured porous aquifer, which accounts for the chemical reactions and fractal geometry of the porous medium.
2. The numerical and analytical solutions will be obtained and asymptotic analysis of these solutions will be carried out. The adequate values of the model parameters will be proposed and validated by comparison with experimental investigations which are in progress now in Tohoku University, Japan.
3. The effect of chemical reactions, fractal dimensions of the porous medium, the anomalous character of the diffusion phenomena, and various flow regimes will be analyzed.

B. Proposed Activities and Timelines

I believe that this grant can help me to develop the reliable mathematical models of reactive contaminant transport and publish these results in the relevant archival journals shortly. These achievements will make my chances in competing for the NSF and Department of Energy grants significantly higher. The results of proposed research can be readily incorporated into my upper division classes "Partial Differential Equations and Boundary Value Problems" and "Mathematical Modeling of Physical Phenomena". Mathematical models and solutions developed within the proposed project will be used as model problems for the NSF REUT grant.

Timetable.

08/15/12- 10/01/12: Based on fundamental laws of mass transport and conservation in a complex fractal medium, the asymptotic governing equations of the contaminant transport will be obtained. The model will be validated and calibrated by comparison with the laboratory and field experiments carried out in Tohoku University, Japan. The problem will be solved analytically and numerically.

10/01/12- 12/31/12; Based on these solutions, the main peculiarities of contaminant dispersion in the porous medium will be assessed and the possible scenarios of the groundwater contamination will be analyzed. The effects of the geological structure and fractal dimension of the medium, the contamination time and dimensions of the aquifer on the possible outcomes of contamination will be considered. The draft of the research paper will be prepared and submitted to the journal of *Applied Mathematical Modeling* or *Transport in Porous Media.*

C. Additional Benefits

In addition to its scholarly significance, the proposed study will also help me to develop a new lecture course "Mathematical Modeling of Physical Phenomena' and to upgrade the teaching material for my class "Partial Differential Equations and Boundary Value Problems". Earning the grant is also important in terms of supporting my research agenda. My productivity as a scholar has gained considerable momentum during the past years, including publication of peer-reviewed articles in 2005 - 2011, textbook, and delivery of several conference presentations. I am collaborating with a number of internationally recognized scientists in several projects that will also result in publications. Receiving the grant will enable me to nurture this momentum, with the following short and long-term benefits:

(a) Enhancing my knowledge and professional development.

(b) Publication of the results in international journals and conferences will help in establishing scientific contacts with researchers from major research universities, will attract new research-oriented faculty to our University, will help me to mentor research of undergraduate students and prepare them for graduate school, and also will contribute to the future development of the Master's degree Program in Applied Mathematics at the Department of Mathematics and Statistics, CSU, Chico.

(c) Relevance to the RTP process. I am currently in my seventh year at CSUC, and obtaining the grant will enable me to work towards the scholarship component of the RTP process.

(d) Increase future possibilities of extra-mural funding from NSF and DOE.