

Final Report for Period: 06/2007 - 05/2008**Submitted on:** 06/06/2008**Principal Investigator:** Goldsztein, Guillermo .**Award ID:** 0505496**Organization:** GA Tech Res Corp - GIT**Submitted By:****Title:**

Mathematical Modeling of Heterogeneous Media

Project Participants**Senior Personnel****Name:** Goldsztein, Guillermo**Worked for more than 160 Hours:** Yes**Contribution to Project:****Post-doc****Graduate Student****Undergraduate Student****Technician, Programmer****Other Participant****Research Experience for Undergraduates****Organizational Partners****Other Collaborators or Contacts**

Guido Kampel, PhD student in the School of Mathematics at Georgia Tech at the time (He graduated in August 2007)

Carlos Santamarina, Professor in the School of Civil and Environmental Engineering at Georgia Tech

Activities and Findings**Research and Education Activities:**

The research objectives are the development of new mathematical tools for the study of the influence of the microgeometry of heterogeneous materials on their macroscopic properties. With those goals in mind, three projects were selected to study: 1) Mechanical properties of composites and polycrystals, 2) Solute transport in porous media and 3) Small particles migration and clogging.

The broad educational objectives are the exposure to students to interdisciplinary work, the development of activities to help students become good modelers, and the participation of students in the research projects of the PI. The educational activities proposed were the development of a course in mathematical modeling of materials and a working seminar in interdisciplinary mathematics.

During the length of the grant (three years) we have obtained very satisfying results in all three projects. As a result, we have published five articles in first rate scientific peer reviewed journals, a sixth article has been submitted for reviewed, three more articles are in preparation and, equally importantly, we have generated several new promising ideas and research directions that we plan pursue. We have presented our results in several conferences and colloquia.

Regarding the educational activities, the PI has organized an interdisciplinary seminar. We were able to have three speakers from the private sector: Heath Herman (KBI BioPharma Inc.) spoke on Centrifugal Bioreactors, Tal Cohen (ClickFox) spoke on a Case Study: The Mathematical Foundations of Business Success and Frederick E Daum (Raytheon Wireless Services) spoke on Nonlinear filters and mathematics. A collaboration has resulted from the talk of Heath Herman. In fact, KBI BioPharma Inc. supported one of our graduate students for a semester to work on a project of their interest and the PI is served as adviser.

Findings:

Findings on the mechanical properties of composites: The yield set of a material is the set of stresses that the material can withstand. We have considered matrix-inclusion composites, i.e. particles (or inclusions) of one (solid) material embedded in a second material called matrix (also a solid). Our goal was to compute the yield set of the composite given the yield set of the inclusions and the matrix, as well as features of the microstructure, i.e. shape, volume fraction and spatial distribution of the inclusions. We restricted our attention to anti-plane deformations and microstructures that allow such deformations. In this context, we were left with a scalar or conductivity two-dimensional problem. We have obtained a bound on the yield set of the composites and shown that that bound is essentially optimal. We have also obtained results on the effect of the shape of the inclusions on the behavior of composites. In particular, we have shown that, while circular inclusions can not strengthen composites much, elliptical inclusions can. This research resulted in three articles that are currently in preparation.

Findings on the transport of solute in porous media: We modeled porous media as a network of interconnected thin channels. We have identified a local physical mechanism that occurs at the intersections of channels and promotes mixing of the solute with the solvent (host liquid). We have also identified the parameter regime where this mechanism is the dominant cause of dispersion and have obtained the effective or macroscopic transport equation that the concentration of solute satisfies. We have also explored the models obtained and gained interesting understanding of the dependence of solute transport on the micro-geometry. This research resulted in three articles that have already appeared.

Findings on the migration of small particles in porous media and clogging: Guido Kampel, a former PhD student in the School of Mathematics at Georgia Tech, has been working with the PI on the study of small particles migration and clogging. These studies lead to Guido's PhD theses that he successfully defended last summer. Professor Santamarina (Civil and Environmental Engineering, Georgia Tech) was also involved in this aspect of the project. He and his research group, has performed a family of experiments that have the goal of providing a better understanding of the global or macroscopic phenomena that lead to the plugging of the porous medium or the migration of fines out of the medium. With Guido Kampel, we have developed the corresponding mathematical models. In addition, we have studied the following problem: We modeled filters as networks of channels. As suspension (fluid with particles) flows through the filter, particles clog channels. We assumed that there is no flow through clogged channels. We have computed a sharp upper bound on the number of channels that can clog before fluid can no longer flow through the filter. This was a very interested result where we have used elements of graph theory and geometry. In particular, our results suggest what micro-geometries lead to efficient filters. This research resulted in two articles that have already appeared and a third one that is currently being reviewed.

Training and Development:

For Guido Kampel (PhD student, Math Gatech), this has been a great research experience. He has done extremely well. He wrote a wonderful PhD dissertation. One third of his dissertation lead to two journal articles: one already published and the other one is currently being reviewed. The rest of his theses will lead to at least two more publications. He became a very good scientist.

Outreach Activities:

Journal Publications

Goldsztein, GH, "Solute transport in porous media: Dispersion tensor of periodic networks", APPLIED PHYSICS LETTERS, p. , vol. 91, (2007). Published, 10.1063/1.276018

Goldsztein, GH, "Volume of suspension that flows through a small orifice before it clogs", SIAM JOURNAL ON APPLIED MATHEMATICS, p. 228, vol. 66, (2005). Published,

Goldsztein, GH, "Transport of nutrients in bones", SIAM JOURNAL ON APPLIED MATHEMATICS, p. 2128, vol. 65, (2005). Published, 10.1137/04061663

Goldsztein, G.H., "Solute transport in porous media. Media with capillaries as voids.", SIAM J. Appl. Math., p. 1203, vol. 68, (2008).
Published,

Kampel, G., Goldsztein, G.H. and Santamarina J.C., " Plugging of porous media and filters: maximum clogged porosity", Appl. Phys. Lett., p. , vol. 92, (2008). Published,

Kampel, G. and Goldsztein, G.H., "Filters. the number of channels that can clog in a network", SIAM J. Appl. Math., p. , vol. , (2008).
Submitted,

Books or Other One-time Publications

Web/Internet Site

URL(s):

www.math.gatech.edu/~ggold

Description:

Other Specific Products

Contributions

Contributions within Discipline:

We have obtained a new bound on the yield set of composites and obtained an understanding on the effect of particle shape on the yield set of composites. These results have a direct impact in the field of composites as well as the mathematical field of homogenization.

We have obtained new and easy to use models to understand the dependence of solute transport in porous media on the micro-geometry of the medium. Our contributions will have an impact in the field of transport in porous media. Our approach resulted from asymptotic expansions where a certain physical phenomenon that we identified is the dominant cause of dispersion. These techniques will also have an impact in the mathematical field of homogenization.

We have developed models to simulate clogging in porous media. This is of importance in the petroleum industry and in filters among others. We have also realized that the tools developed during the first year can be used to study other transport phenomena in porous media. In particular, heat and reactive transport in porous media can be studied with our methods. This is of importance to understand the transport of contaminants in soils.

All our results have impacts in the general field of applied mathematics and applied physics.

Contributions to Other Disciplines:

Our results will also impact several fields. These include: 1) Material Science and Engineering, where the understanding of the mechanical properties of composites is important; 2) Bio-Engineering and Bio-Mechanics, since understanding transport of solute in porous media is essential to the understanding of transport of nutrients in bones; 3) Environmental Engineering, since both the transport of solute as well as the migration of fines and clogging in porous media play fundamental roles in the transport of contaminants in soils; 4) Filters, etc. Thus, potential applications include new guidelines on the design of new composites, on the disposal of contaminants, the design of improved methodologies to treat osteoporosis and related diseases, a better understanding of the processes that lead to loss of bone experienced in the absence of gravity (during space flights) and improve methodologies for bone implants.

Contributions to Human Resource Development:

Contributions to Resources for Research and Education:

Contributions Beyond Science and Engineering:

Categories for which nothing is reported:

Organizational Partners

Activities and Findings: Any Outreach Activities

Any Book

Any Product

Contributions: To Any Human Resource Development

Contributions: To Any Resources for Research and Education

Contributions: To Any Beyond Science and Engineering