

# Highly Filled Materials Institute at Stevens

# NEWS

Spring 2002

## 13th ANNIVERSARY ISSUE

### From the Director

Dear Friends:

**This year** we are celebrating the 13<sup>th</sup> anniversary of the founding of HfMI. Our Research Center grew in many directions during the last two years and the number of our sponsors reached sixty. We are proud that you have selected us as your research and development partner and have trusted us with some of your most challenging problems and tasks.

Our scope of activities grew with the increasing number of projects received. We developed comprehensive facilities and know-how in particle formation and characterization, rheology, simulation and processing, structure development, and quality control and the tailoring of the ultimate properties of a wide variety of materials. These include explosives, solid rocket fuels, propellants and pyrotechnic materials, battery suspensions, personal care products, toners, inks, encapsulation materials for electronic packaging, thermal greases for chips, and food products.



### INFRASTRUCTURE

We use state-of-the-art SGI machines with multiple parallel processors to run our 3-D FEM-based source codes. Over 50 of our computers are linked to a central file server which also serves as our archive. The archive contains a digital library with our papers, reports, key lectures, procedures, designs, source codes, and manuals. This work required many months of dedicated effort on a myriad of tasks and thanks go to Mr. Kiryaman and his associates who made this happen. On the experimental side, we have increased our capabilities by designing and building a shear roll mill pilot facility and new types of extrusion dies, rheometers and

extruders. These can be used with our new thermal and high-speed cameras. We now have the tools necessary for the mathematical-modeling-based custom design of novel sensors, rheometers, dies, and processing equipment. Through our industrial partners, such tools can be manufactured and delivered to our sponsors. Our capabilities will increase further with the installation of the new Universal Extrusion System in our processing lab (*see top of page 3*).

### MATHEMATICAL MODELING

Simulation at HfMI starts with the mathematical modeling of the particle formation processes, including deposition of nano particles from the vapor phase and crystallization from solution and goes all the way to mixing and processing of various highly filled material formulations occurring in continuous processors in very complex geometries. The leadership and diligent work of Dr. Ralph Schefflan and Dr. Moinuddin Malik in simulation deserve special recognition. In the area of mathematical modeling of continuous processing operations we now have the ability to solve the conservation equations to determine the temperature, stress, residence time and velocity distributions for the entire single- or twin-screw extruder and die combination. This provides realistic solutions to industry and Department of Defense organizations in the processing of complex materials, including the processing of energetic materials.

### TECHNOGENESIS

During the last three years, the educational and research mission of SIT has been reorganized around a new strategic direction, Technogenesis<sup>®</sup>, i.e., the development and commercialization of new technologies. There is now even a popular Technogenesis TV talk show hosted by our President Dr. Harold J. Raveché which just marked its first anniversary (for more information visit [www.technogenesis.tv](http://www.technogenesis.tv)). HfMI has been contributing to this effort by working together with Material Processing and Research, Inc. (MPR) of Hackensack, NJ, which is headed by James B. Graybill. Some of you will know Jim from his days at the helm of Baker Perkins Inc. of Saginaw, Michigan. Jim can be contacted at 201-525-1312 for addressing your needs in the development of new sensors, extruders, dies, devices, rheometers and novel materials.

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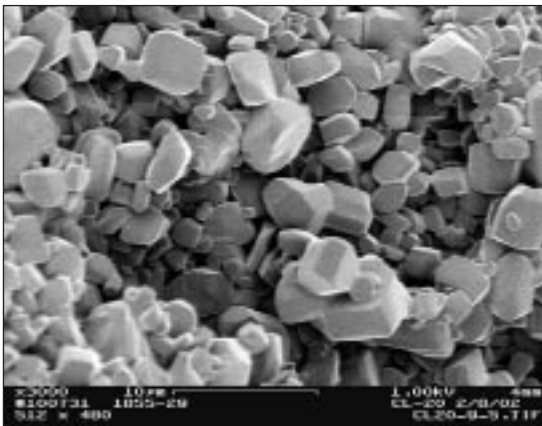
# Projects

## ■ SHEAR ROLL MILLING OF GUN PROPELLANTS

This project aims at generating a fundamental understanding of the shear roll mill process. As part of this project we have carried out experiments at the NitroChemie facility in Aschau, Germany using a double base gun propellant. The team in Germany included Messrs. Shah and Gevgilili of HfMI, Mr. Hays Zeigler of Alliant, Messrs Rosenberg, Topolski, and Ms. Campesi of the US Army.

As part of the project we have designed and, through our partnership with Shear Tool Inc. of Saginaw, Michigan, manufactured a complete pilot shear roll mill facility. This is an 85 mm machine which is used both to understand the basic mechanisms of the shear roll mill process and to validate our mathematical models of the process. Our project partners are the TACOM/ARDEC of US Army and Alliant-Tech Systems of Radford, Virginia.

*Photo: the Shear Roll Mill pilot facility of HfMI*



## ■ COATING THICKNESS DETERMINATION OF CL-20

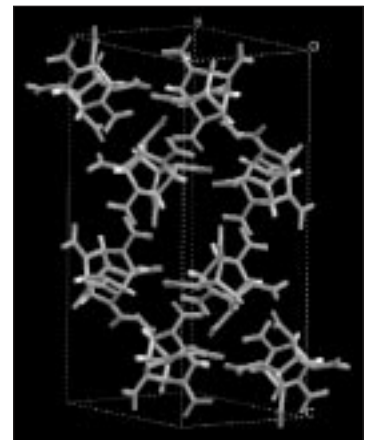
The coating thickness distribution affects the sensitivity and other ultimate properties of energetic materials. We aim to develop a new technique based on the glancing x-ray analysis to determine the coating thickness of slurry coated CL-20 crystals. The technologies developed will be used for on-line analysis of the coating thickness distributions of slurry coated particles. Our project partners are the TACOM/ARDEC of the US Army and the Thiokol Aerospace Division of Alliant-TechSystems.

## ■ EXTRUSION OF Mg-BASED FLARE COMPOSITIONS, BAMO/AMMO FORMULATIONS AND LOVA's

In the energetics processing arena we have been busy with multiple projects involving explosives, propellants and pyrotechnics. Our work in these areas was sponsored and partnered by TACOM/ARDEC and the Indian Head Division of the Naval Surface Warfare Center. The projects involved analysis of rheological characterization data, mathematical modeling, simulant development, analysis of the structural distributions in processed grains, and design of hardware including multi strand dies.

## ■ MODEL-BASED CONTROL OF CRYSTALLIZATION PROCESSES FOR ENERGETIC PARTICLES

This project aims at incorporating model-based process control to the facilities used for the crystallization of RDX at U.S. Army's Holston facility. Our project partners are TACOM/ARDEC of the US Army and BAE Systems.



## ■ CONCEPT DESIGN FOR FLEXIBLE MANUFACTURING OF ENERGETIC MATERIALS

This project aims to develop the working principles and the basic design concepts for the next generation of plants for the manufacturing of energetic materials. The next generation facilities will utilize rigorous material characterization with comprehensive mathematical models of the processes

## New Staff

involved in the manufacture of energetic materials; starting with the nitration reactions, and followed by the crystallization processes, mixing, devolatilization, pressurization of the energetic suspensions, their shaping into grains and on-line quality control. Mathematical-modeling-based selection of the modular elements to define each processing step renders such facilities truly flexible and economically possible. For example, one such flexible processing unit is the Universal Extrusion System of HfMI. This is a single extrusion platform (one single set of feeders, gear box, motor etc.), which has the ability to function as a single screw or twin screw (co-rotating, counter-rotating extruder in the non-intermeshing, or partially-intermeshing or the fully-intermeshing modes) or a shear roll mill.

### ■ MANUFACTURING OF SOAP BARS

We have continued to carry out projects funded by the non-defense industries in the general areas of rheology, simulation, experimental processing studies, structural analysis and tool design. Recently we completed a five year investigation for Unilever in the area of manufacturing of soap formulations. The project included mathematical modeling of the processing of soap bars in single and twin screw extruders, the development of the microstructure of soap during its flow and deformation and the rheological behavior as affected by the ingredients of the formulation. Our techniques allow the development of personal care products concurrent with predictions of their processability at the plant level.

### ■ MANUFACTURING OF ENCAPSULATION MATERIALS

In the area of encapsulation materials for the electronics industry, we have started to work with Henkel Loctite of Olean, NY. This multinational company is a leading supplier of semiconductor and electronic component encapsulating materials. Our project aims at developing the next generation manufacturing base for the mixing and processing of these materials.

**We are** very pleased that a special group of dedicated and very capable scientists joined our research center. They include:

**Dr. Hasan Gocmez** Dr. Gocmez received his PhD degree in ceramic and materials science and engineering from Rutgers University in New Jersey. He is specializing in the areas of crystallization and structural analysis.

**Dr. Berton Greenberg** Before joining the Highly Filled Materials Institute as a senior research scientist, Dr. Berton Greenberg worked as materials characterization group leader and senior member of research staff with over 15 years of industrial experience in structural characterization of electronic and other materials for research and manufacturing. He is a recognized leader in x-ray diffraction with over 50 published papers and presentations.

**Dr. Moinuddin Malik** Dr. Moinuddin Malik received his PhD degrees in Mechanical Engineering from University of Roorkee and University of Oklahoma. Prior to joining HfMI as a senior research scientist, he worked at New Jersey Institute of Technology, NASA Langley Research Center and University of Oklahoma. Dr. Malik has significant expertise in computational methods, as well as granular mechanics, with over 80 published papers and presentations.

**Dr. Ralph Schefflan** Dr. Schefflan received his PhD from Columbia University in chemical engineering and is an adjunct professor of chemical engineering at SIT. His previous experience includes serving as the Head of the Process Control Group at Hoffmann-LaRoche. His industrial expertise and simulation skills are currently significant assets of HfMI.

**Dr. Hansong Tang** Similar to Dr. Malik, Dr. Tang also received two PhD degrees in engineering and applied mathematics from China and Georgia Institute of Technology. He is currently working in the area of mathematical modeling of various manufacturing operations at HfMI.

HfMI is also fortunate to be served well by the diligent and enthusiastic efforts of a talented group of new research assistants. They include Messrs. Anand Shah, Manaf Zghaibeh, Matin Shaikh, Guangyu Lu, Levent Karakas, Dharmesh Dalwadi and Ms. Melek Erol and Ms. Trusha Sanghvi.

## Milestones



### Dr. Rahmi Yazici

We at HfMI continue to feel the loss of our dear friend and colleague, Dr. Yazici, who passed away in February 2000. Rahmi was a very creative researcher who tirelessly developed various technologies in the areas of structural analysis and characterization, especially using x-ray techniques. He will always be missed.

### Retirement of Kathy Norman

Ms. Norman retired from her position as the administrative assistant of HfMI. We will miss Kathy's cheerful greetings and her organizational skills. We all thank Kathy for 10 years of service to HfMI and wish her well in her retirement.

# Recent Publications and Presentations

## Publications and available manuscripts since the last newsletter:

H. Gevgjilli and D. M. Kalyon, "Catastrophic Failure of the No-Slip Condition at the Wall during Torsional Flows and the Development of Gross Surface Irregularities During Capillary Flow of Three Polymers," submitted to *SPE ANTEC Technical Papers*, November (2001).

D. M. Kalyon, E. Birinci, B. Karuv and S. Walsh, "Electrical Conductivity of a Graphite Based Composite as Affected by the Degree of Mixedness of Graphite in the Elastomeric Matrix," submitted to *SPE ANTEC Technical Papers*, November (2001).

H. Gevgjilli and D. M. Kalyon, "Effect of Wall Slip of Polymer Melts on Their Relaxation Modulus Behavior," submitted to *SPE ANTEC Technical Papers*, November (2001).

D. M. Kalyon, E. Birinci and B. Karuv, "Electrical Properties of Conductive Composites as Affected by the Degree of Mixedness of the Conductive Filler in the Polymer Matrix," accepted to appear in *Polym. Eng. Sci.* (2002).

A. Wagner, D. M. Kalyon, R. Yazici, and T. Fiske, "Uniaxial Extensional Flow Behavior of a Glass Fiber-Filled Engineering Plastic," accepted to appear in *Journal of Reinforced Plastics and Composites*, November 2001.

H. Gevgjilli and D.M. Kalyon, "Step Strain Flow: Wall Slip and other Error Sources," *J. Rheology*, 45, 2, 467-475 (2001).

Dilhan M. Kalyon, "Rheological Behavior of Concentrated Suspensions," *Proceedings of Polymer Processing Society Regional Meeting*, Pages 51-52, October 22, 2001.

Dilhan M. Kalyon, "Extrusion of Highly Filled Materials: Rheology, Structure Development, Mathematical Modeling and Experimental Studies," *Polymer Processing Society Regional Meeting*, Pages 199-200, October 22, 2001.

Dilhan M. Kalyon, "New Developments in Rheological Characterization of Energetic Materials," *Proceedings of the 11th Joint Ordnance Commander's Group, Continuous Mixer and Extruder Users Group Meeting*, Picatinny Arsenal, Dover NJ on May 2, 2001.

Dilhan M. Kalyon, "Continuous Processing of Energetic Materials," *Proceedings of the 11th Joint Ordnance Commander's Group, Continuous Mixer and Extruder Users Group Meeting*, Picatinny Arsenal, Dover NJ on May 2, 2001.

A. Lawal, S. Raikar and D. M. Kalyon, "Mathematical Modeling of Three-Dimensional Die Flows of Viscoplastic Fluids with Wall Slip," *Journal of Reinforced Plastics and Composites*, 19, 18, 1483-1492 (2000).

M. Allende and D. M. Kalyon, "Assessment of Particle-Migration Effects in Pressure-Driven Viscometric Flows," *J. Rheology*, 44, 1, 79-90 (2000).

A. Lawal and D. M. Kalyon, "Compressive Squeeze Flow of Viscoplastic Fluids with Apparent Wall Slip," *International Polymer Processing*, 15, 1, 63-71 (2000).

D. M. Kalyon, A. Lawal, R. Yazici, P. Yaras and S. Raikar, "Mathematical Modeling and Experimental Studies of Twin Screw Extrusion of Filled Polymers," *Polym. Eng. Sci.*, 39, 6, 1139-1151 (1999).

D. M. Kalyon, S. Raikar and A. Lawal, "New techniques for the Simulation of the Die and Twin Screw Extrusion Processing of Energetic Materials," *Proceedings of the 10th Joint Ordnance Commander's Group, Continuous Mixer and Extruder Users Group Meeting*, Thiokol Center, Brigham City, Utah, 1999, pages 14-39.

J. E. Kowalczyk and D. M. Kalyon, "Simulation Based Design and Manufacture of Screws and Dies for the Energetics Industry," *Proceedings of the 10th Joint Ordnance Commander's Group, Continuous Mixer and Extruder Users Group Meeting*, Thiokol Center, Brigham City, Utah, 1999, pages 40-60.

R. Yazici and D. M. Kalyon, "On-Line and Off-line Analysis of the Extruded and Cast Energetic Materials for Microstructural Distributions," *Proceedings of the 10th Joint Ordnance Commander's Group, Continuous Mixer and Extruder Users Group Meeting*, Thiokol Center, Brigham City, Utah, 1999, pages 61-69.

M. Gallant, W. Newton, S. Johnson, S. Prickett, D. M. Kalyon, A. Lawal and S. Raikar, "Twin Screw Processing of GEM Gun Propellant," *Proceedings of the 10th Joint Ordnance Commander's Group, Continuous Mixer and Extruder Users Group Meeting*, Thiokol Center, Brigham City, Utah, 1999, pages 88-96.

T. Fiske, H. S. Gokturk, R. Yazici and D. M. Kalyon, "Relative Magnetic Permeability of Injection Molded Composites as Affected by the Flow Induced Orientation of Ferromagnetic Particles," in *Imaging and Image Analysis Applications of Plastics*, B. Pourdeyhimi ed., ChemTec Publishing (1999).

## Theses since the last newsletter:

Melquiades Allende, "Shear Induced Particle Migration in Suspensions of Non-Colloidal Particles," PhD Thesis, Stevens Institute of Technology, Hoboken, NJ.

Louisa M. Lao, "Dynamics of Crystallization and Properties of Organic Crystals," PhD Thesis, Stevens Institute of Technology, Hoboken, NJ.

Elvan Birinci, "Characterization of the Degree of Mixedness of Composites and Correlations with Ultimate Properties," Master of Engineering Thesis, Stevens Institute of Technology, Hoboken, NJ.

Ali Arslantas, "Crystallization and Structural Analysis by X-ray Diffraction in Organic Crystals," PhD Thesis, (supervised by Prof. W. Ermler) Stevens Institute of Technology, Hoboken, NJ.

Esra Kucukpinar, "Shear and Extensional Flows of Metallocene-Catalyzed Polyethylenes and Novel Thermoplastic Elastomers," Master of Engineering Thesis, Stevens Institute of Technology, Hoboken, NJ.

Halil Gevgjilli, "Shear Viscosity and Extrudability of a Soap Formulation," Master of Engineering Thesis, Stevens Institute of Technology, Hoboken, NJ.

The PhD theses of Messrs. Guangyu Lu and Halil Gevgjilli should also be completed and available by May 2002.

## Presentations since the last newsletter:

D. M. Kalyon, "Rheology and Extrusion of Highly Filled Polymeric Suspensions," Massachusetts Institute of Technology, *Program in Polymer Science and Technology Seminar*, October 31, 2001.

Dilhan M. Kalyon, "Rheological Behavior of Concentrated Suspensions," *Keynote Lecture, Polymer Processing Society Regional Meeting*, October 22, 2001.

Dilhan M. Kalyon, "Extrusion of Highly Filled Materials: Rheology, Structure Development, Mathematical Modeling and Experimental Studies," *Polymer Processing Society Regional Meeting*, October 22, 2001.

D. M. Kalyon, "Extrusion of Pastes and Soft Solids," *2001 IFPRI Annual General Meeting*, Gainesville, Florida, July 11, 2001.

Dilhan M. Kalyon, "New Developments in Rheological Characterization of Energetic Materials," *Joint Ordnance Commanders Group 11th Continuous Mixer and Extruder Users Group Meeting*, Picatinny Arsenal, Dover NJ on May 2, 2001.

Dilhan M. Kalyon, "Continuous Processing of Energetic Materials," *Joint Ordnance Commanders Group 11th Continuous Mixer and Extruder Users Group Meeting*, Picatinny Arsenal, Dover NJ on May 2, 2001.

R. Schefflan, S. Kovenkloglu and D. M. Kalyon, "Modeling of Aluminum Nanoparticle Formation," *199th Meeting of the Electrochemical Society on March 27, 2001 in the Fundamental Gas-Phase and Surface Chemistry of Vapor Deposition II and Process Control, Diagnostics and Modeling Symposium*, Washington, DC.

D. M. Kalyon, "Rheology and Processing of Highly Filled Suspensions," Duracell Bethel Corporate Facility, November 2, 2000.

D. M. Kalyon, "Extrusion of Pastes and Soft Solids," *2000 IFPRI Annual General Meeting*, Scheveningen, Den Haag, The Netherlands, July 11, 2000.

D. M. Kalyon, "Improvement of Extrusion Process Efficiency," Dexter Electronic Materials, Olean, NY, June 12, 2000.

D. M. Kalyon, "Structure and Processing of Highly Filled Materials," Eugenie Lamothe Colloquium Series, Department of Chemical Engineering of McGill University, January 24, 2000.

D. M. Kalyon, "Rheology, Structure Development/Characterization and the Simulation of the Extrusion Processing of Highly Filled Materials," Duracell-Gillette Company, Needham, Massachusetts, January 10, 2000.

D. M. Kalyon, "Mathematical Modeling of the Continuous Processing of Highly Filled Materials," Seminar Series in Applied Mathematics, Department of Mathematical Sciences at Stevens Institute of Technology, December 6, 1999.

D. M. Kalyon, "Simulation of the Extrusion of Soap Formulations," Unilever Edgewater Research and Development, Edgewater, NJ November 29, 1999.

D. M. Kalyon, "Viscoelasticity of ink formulations and Ramifications on Misting of uv-curable inks," Sun Chemical, Carlstadt, NJ, October 29, 1999.

D. M. Kalyon, "Processing of Highly Filled Materials and Applications to Co-extruded Permanent Magnets," Delphi Automotive Systems, Saginaw, Michigan, Sept. 24, 1999.

D. M. Kalyon, "New Concepts in Casting of Rocket Fuels," Naval Surface Warfare Center, Indian Head, Maryland, Sept. 21, 1999.

D. M. Kalyon, "Continuous Processing of Highly Filled Materials: Possible Applications to Processing of Pulp and Paper Waste Products," Marcal Paper Mills Inc. Elmwood Park, NJ, Aug. 11, 1999.

D. M. Kalyon, "Extrusion of Pastes," *IFPRI Annual Meeting*, New Brunswick, NJ, June 8, 1999.