



**Chemical  
Engineering**



**2005-2006**

**RESEARCH BROCHURE**





## MESSAGE FROM THE CHAIR

Our research directions revolve around three major areas within chemical engineering: *process systems engineering*, *polymer science and engineering*, and *bioengineering*. These research areas are linked to the undergraduate curriculum so that our students can benefit from the research expertise within the Department and meet the vision of the University's Academic Plan. Graduate Students in the M.A.Sc. and Ph.D. program have access to a selection of Graduate courses in these areas, as well as exceptional research equipment.

The five-year undergraduate program *Chemical Engineering and Bioengineering* provides the full chemical engineering undergraduate experience, combined with an additional year of study in the life sciences, anatomy, biochemistry and bioengineering electives. The program is intended to provide opportunities for students to broaden their knowledge beyond the traditional chemistry and physics based components of chemical engineering science with further study of the biological sciences. We offer a four year *Chemical Engineering* program and the five year *Chemical Engineering and Management* and *Chemical Engineering and Society* programs. The existing programs have been enhanced with the addition of groups of courses linked to the research strengths of the Department. The *Process Systems and Engineering stream* provides enrichment electives in the areas of process control, simulation and statistics. The *Polymer Materials and Manufacturing stream* provides enrichment technical electives in the areas of polymer science, processing and reactor engineering and will be the opening to the combined *Bachelor's and Master's program in Manufacturing Engineering*. Professional graduate degrees are offered in the School for Engineering Practice with three Master Programs in *Engineering Entrepreneurship and Innovation*, *Engineering and Public Policy* and *Design*.

Dr. Shiping Zhu, Dr. Raja Ghosh and Dr. Bob Pelton have been awarded *Canada Research Chairs*, in recognition of their outstanding research achievements and promise for future discoveries. We also have two faculty designated as *Distinguished University Professors*, Drs John Brash and John MacGregor – the highest rank awarded at the University that recognizes outstanding academic contributions.

If you have any comments, questions or just want to find out more about us, please contact me and I'll be glad to tell you more.

Andrew Hrymak,  
Professor and Chair  
September, 2005

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## FACULTY AND STAFF

### FACULTY

- Dickson, J.M. B.A.Sc., M.A.Sc. (Waterloo), Ph.D. (Virginia Polytech. Inst. & State Univ.)  
*Professor*
- Filipe, C. B.S. (Escola Superior de Biotecnologia, Portugal), Ph.D. (Clemson)  
*Assistant Professor*
- Ghosh, R. B.S., M.S. (Jadavpur University, India), D.Phil. (Oxford).  
*Assistant Professor*
- Hrymak, A.N. B.Eng. (McMaster), Ph.D. (Carnegie Mellon), P.Eng.  
*Professor and Chair*
- Jones, K.J. B.A.Sc. (Waterloo), M.Sc. (Guelph), Ph.D. (Toronto)  
*Assistant Professor*
- Loutfy, R. M.Sc, B.Sc, (Ain Shams University) Ph.D, (Western)  
MBA (Toronto)  
*Professor*
- MacGregor, J.F. B.Eng. (McMaster), M.S., Ph.D. (Wisconsin), FASA, P.Eng.  
*Distinguished University Professor*
- Marlin, T.E. B.S. (SUNY at Buffalo), M.S. (Dayton), Ph.D. (Massachusetts)  
*Professor*
- Mhaskar, Prasant B.T. (IIT) M.S. (Louisiana) Ph.D. (UCLA)  
*Assistant Professor*
- Pelton, R.H. B.Sc., M.Sc. (Guelph), Ph.D. (Bristol)  
*Professor*
- Sheardown, H. B.Eng. (McMaster), Ph.D. (Toronto), P.Eng.  
*Associate Professor*
- Swartz, C.L.E. B.Sc. (Cape Town), Ph.D. (Wisconsin-Madison)  
*Associate Professor*
- Taylor, P.A. B.Sc., Ph.D. (North Wales), P.Eng.  
*Professor (Joint with Computing and Software)*

Thompson, M.R. B.Sc., B.Eng., M.Eng. (McMaster), Ph.D. (Waterloo)  
*Assistant Professor*

Vlachopoulos, J. Dipl. Chem. Eng. (National Tech. Univ. of Greece), M.S., D.Sc.  
(Washington, St. Louis), F.C.I.C., P.Eng.  
*Professor*

Wood, P.E. B.A.Sc. (Waterloo), Ph.D. (Caltech), F.C.I.C., P.Eng.  
*Professor, Associate Vice-President, Student Affairs*

Zhu, S. B.Eng. (Zhejiang), Ph.D. (McMaster), P.Eng.  
*Professor (joint with Materials Science & Engineering)*

### **EMERITUS FACULTY**

Baird, M.H.I. B.Sc., (Glasgow); Ph.D., (Cambridge), F.C.I.C., P.Eng.  
*Emeritus Professor*

Brash, J.L. B.Sc., Ph.D. (Glasgow), Dhon.Caus. (Paris Nord), P.Eng.  
*Distinguished University Professor*  
*Director, McMaster School of Biomedical Engineering*

Crowe, C.M. B.Eng. (McGill); Ph.D. (Cambridge), F.C.I.C.  
*Emeritus Professor*

Feuerstein, I.A. B.Chem.Eng. (City College of New York), M.S. (Newark College  
of Eng); Ph.D. (Massachusetts)  
*Emeritus Professor*

Hamielec, A.E. B.A.Sc., Ph.D. (Toronto), F.R.S.C., F.C.I.C., P.Eng.  
*Emeritus Professor*

Shemilt, L.W. O.C., B.A.Sc., Ph.D. (Toronto), M.Sc. (Manitoba), D.Eng.  
(Waterloo), D.Hon.C (Kracow), D.Sc. (McMaster, F.R.S.C.,  
F.C.A.E., F.C.I.C., F.A.I.ChE., F.E.I.C., P.Eng.  
*Emeritus Professor*

Woods, D.R. B.Sc. (Queen's), M.Sc., Ph.D. (Wisconsin), D.Sc. (Queen's,  
Guelph), F.C.I.C., F.A.I.Ch.E., P.Eng.  
*Emeritus Professor*

## **ADJUNCT FACULTY**

Jones, L.	B.Sc. (Wales) Ph.D. (Aston) <i>Associate Professor</i>
Kostanski, K.	M.Eng., Ph.D. (Technical University of Szczecin) <i>Assistant Professor</i>
Kourti, D.	Dipl. Eng. (Chemical) (Aristotle Univ., Greece), Ph.D. (McMaster) <i>Associate Professor</i>
Quinn, S.	B.Sc., B.A.Sc. (Ottawa), Ph.D. (Queen's) <i>Assistant Professor</i>
Wright, J.D.	B.Sc. (Alberta), Ph.D. (Cambridge), P.Eng. <i>Professor</i>

## **ASSOCIATE MEMBERS**

Brook, M.A.	B.Sc. (Toronto), Ph.D. (McGill), M.C.I.C. <i>Professor of Chemistry</i>
Dalnoki-Veress, K.	B.Sc., M.Sc., Ph.D. (Guelph) <i>Assistant Professor of Physics and Astronomy</i>
Kevlahan, N.	B.Sc. (British Columbia), Ph.D. (Cambridge) <i>Assistant Professor of Mathematics and Statistics</i>
McDermid, J. R.	B.Sc. (Queen's) M. Eng. Ph.D. (McGill) <i>Associate Professor</i>
West-Mays, J.	H.B.Sc. (Wilfrid Laurier) Ph.D. M.Sc. (Waterloo) <i>Associate Professor</i>

## **VISITORS (2003-04)**

Feng, Zhinan	Institute of Paper Science & Technology, U.S.A.	(R. H. Pelton)
Li, Sara	Zhengzhou Univ., China	(A. N. Hrymak)
Peyaud, Franck	I.S.T.L. France	(A. N. Hrymak)

## **POSTDOCTORAL FELLOWS**

Apostolou, Kostas	Univ. of Minnesota	(A. N. Hrymak)
Dai, Sheng	Nanyan Tech. Univ. Singapore	(R. H. Pelton)
Gorbert, Maud	Univ. Toronto	(K.Jones/H.Sheardown)
Krump, Henrich	Slovak Univ. Technology	(M. Thompson)
Li, ChenSha	Tsinghua Univ. China	(R. Loutfy)
Li, Xin.	Kyushu University Japan.	(R. H. Pelton)

## **TECHNICAL STAFF**

Cornelius, Rena	Research Assistant	(J.L. Brash)
Derkach, Justyna	Undergraduate Lab and Research Assistant	
Dunn, Kevin	Res. Engineer	(MACC)
Hanumanth, Gurumkonda	Res. Engineer	(A. N. Hrymak)
Gatt, Paul	Technician/Machinist	
Keller, Doug	Lab Manager	(Dept./R.H. Pelton/A.E. Hamielec)
Kostanski, Kris	Research Scientist	(A.E. Hamielec/J.F. MacGregor)
Liu, Lina	Research Associate	(H. Sheardown)
McClung, Glenn	Research Assistant	(J.L. Brash)
Nadella, Venkata	Research Associate	(A.N.Hrymak)
Slater, Gord	Technical Services Coordinator	
Takacs, Elizabeth	Lab Manager	(MMRI)
Yu Honglu	Research Engineer	(J. F. MacGregor)

**OFFICE STAFF**

Falkiner, Lynn

Departmental Secretary

Goodram, Kathy

Administrative Coordinator

Vickers, Andrea

Graduate Secretary

## CHEMICAL ENGINEERING FACULTY

### **BAIRD, MALCOLM H.I. (Professor, Emeritus)**

**Research Interests:** reciprocating-plate columns, transport phenomena, mixing and the extraction/refining of non-ferrous metals.



### **Professional Organizations**

Member:

- Association of Professional Engineers of Ontario
- Chemical Institute of Canada

### **Papers in Refereed Journals**

M.Zaki, I.Nirdosh, M.H.I.Baird , and G.H.Sedahmed, "Effect of Superimposed Pulsating Flow on Liquid-solid Mass Transfer in Fixed Beds" Can. J. Chem Eng., in press (2005).

M. Zaki, I. Nirdosh, G.H. Sedahmed and M.H.I. Baird, "Liquid-solid Mass Transfer in Packed Beds" Chem. Eng. & Tech., 27, 414-416 (2004).

P. A. Moysey, M. H. I. Baird and N. V. Rama Rao "Size Segregation of Nickel Pellets Flowing into a Packed Bed" Can. J. Chem. Eng., 82, 424-432 (2004).

M.H.I.Baird and N.V.Rama Rao, "Gas-Liquid Mass Transfer in a 15 cm diameter Reciprocating Plate

Column", J.Chem.Technol.Biotechnol. 77,1-4 (2003).

X.Ni, M.R.Mackley, A.P.Harvey, P.Stonestreet, M.H.I.Baird and N.V.Rama Rao, "Mixing through Oscillations and Pulsations -- a Guide to achieving Process Enhancements in the Chemical and Process Industries" Chem.Eng.Research & Design , 81, 373-383 (2003).

M.H.I. Baird and N. V. Rama Rao, "Gas Liquid Mass Transfer in a 15 cm diameter Reciprocating Plate Column", presented at Engineering Foundation Conference on Process Innovation and Process Intensification, Edinburgh, Scotland, Sept 9-13 (2002)

T. C. Lo and M.H.I.Baird "Liquid-Liquid Extraction" Encyclopedia of Physical Science and Technology, Academic Press, 3<sup>rd</sup> edition, 15, 341-362 (2002)

M.H.I.Baird and N.V.Rama Rao, "Optimum Bottom-Stirring in a Horizontal Cylindrical Vessel", Can. J. Chem. Eng., 79, 609-696 (2001).

X.Ni., Y.S.de Gélécourt, M.H.I.Baird and N.V.Rama Rao, "Scale-up of Single Phase Axial Dispersion in Batch and Continuous Oscillatory Baffled Tubes", Can. J. Chem. Eng., 79, 444-448 (2001).

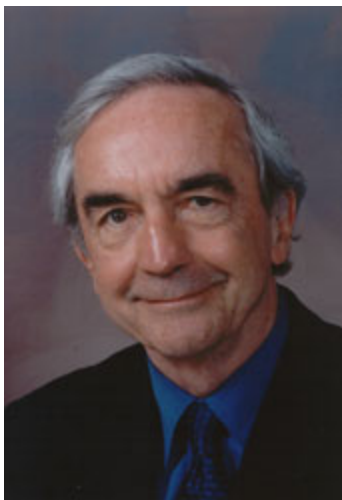
M.H.I.Baird and I.Nirdosh, "Low-Cost Experiments in Mass Transfer: Part 8. Absorption of Carbon Dioxide from a Single Gas Bubble" Chem. Eng. Educ. 35, 198-201 (2001).

### **Current Research Project**

*Dr. Baird is interested in oscillatory flow effects and also in the extraction/refining of non-ferrous metals. As of 2005 he has one experimental project on heat transfer to a moving packed bed of nickel pellets.*

## BRASH, JOHN L. (University Professor)

**Research Interests:** biomaterials, biocompatibility, blood-material interactions, blood compatible materials, surface modification of polymers, free radical and condensation polymerization.



## Professional Organizations

Fellow, Royal Society of Canada

Member:

- Association of Professional Engineers of Ontario
- Canadian Biomaterials Society

## Papers in Refereed Journals

A.P. Hitchcock, C. Morin, X. Zhang, T. Araki, J. Dynes, H. Stover, J.L. Brash, J.R. Lawrence, G.G. Leppard, "Soft X-ray spectromicroscopy of biological and synthetic polymer systems", *J. Electron Spectroscopy*, 144-147, 259-269 (2005).

L.D. Unsworth, H. Sheardown, J.L. Brash, Protein resistance of surfaces prepared by sorption of end thiolated poly (ethylene glycol) to gold: Effect of surface chain density. *Langmuir* 21: 1036-1041 (2005).

L.D. Unsworth, Z. Tun, H. Sheardown and J.L. Brash, Chemisorption of thiolated poly (ethylene oxide) to gold: surface chain densities measured by ellipsometry and neutron reflectometry. *J Colloid Inter Sci* 281: 112-121 (2005).

J. G. Archambault, and J. L. Brash, "Protein repellent polyurethane-urea surfaces by chemical grafting of PEO: amino-terminated PEO as grafting reagent" *Colloids Surfaces B: Biointerfaces*, 39, 9-16 (2004).

C. Morin, A.P.Hitchcock, R. M. Cornelius, J. L. Brash ,S.G. Urquhart, A. Scholl and A.Doran, "Selective adsorption of protein on polymer surfaces studied by soft X-ray photoemission electron microscopy". *J. Electron Spectroscopy*, 137-140, 785-794 (2004).

W.Feng, J. L. Brash, and S.Zhu, "Atom-Transfer Radical Grafting Polymerization of 2-Methacryloyloxyethyl Phosphorylcholine from Silicon Wafer Surfaces". *J Polymer Sci Polymer Chem*, 42, 2931-2942 (2004).

A. Jahangir, C.McCloskey, W.G. McClung, J. L. Brash, R.S. Labow, J.P. Santerre. The influence of protein adsorption and surface modifying macromolecules on the hydrolytic degradation of a polyether-urea-urethane by cholesterol esterase, *Biomaterials*, 24, 121-130 (2003).

Y.J.Du, and J. L. Brash "Synthesis and characterization of thiol-terminated poly(ethylene oxides) for chemisorption to gold surface". *J Appl. Polymer Sci*, 90, 594-607 (2003).

W.G. McClung, D.L. Clapper, A.B. Anderson, D.E.Babcock, and J.L. Brash, "Interactions of fibrinolytic system proteins with lysine-containing surfaces". *J. Biomed Mater Res.*, 66A, 795-801 (2003).

R. M.Cornelius, J. Sanchez, P.Olsson, and J. L. Brash, "Interactions of antithrombin and proteins in the plasma contact activation system adsorbed on immobilized functional heparin". *J. Biomed Mater. Res.*, 67A, 475-83 (2003).

A.R. Jahangir, W.G. McClung, R. M. Cornelius, C.B. McCloskey, J. L. Brash, J.P. Santerre, "Fluorinated surface modifying macromolecules: modulating adhesive protein and platelet interactions on a polyether-urethane", *J Biomed Mater Res.*, 60, 135-147 (2002).

R. M. Cornelius, J.G Archambault, and J.L. Brash,. "Identification of apolipoprotein A-I as a major adsorbate on biomaterial surfaces after blood or plasma contact". *Biomaterials*, 23, 3583-3587 (2002).

A.P. Hitchcock, C. Morin, Y.M.Heng, R. M. Cornelius and J. L. Brash "Towards soft X-ray spectromicroscopy of biomaterials". J. Biomat. Sci. Polymer Edn., 13, 919-938 (2002).

J.M. Van Raamsdonk, R. M. Cornelius, J. L. Brash, and P. L. Chang, "Deterioration of polyaminoacid-coated alginate microcapsules *in vivo*". J. Biomat. Sci. Polymer Edn., 13, 863-884 (2002).

R.M. Cornelius, W.G. McClung, R.M.A. Richardson, C. Estridge, N. Plaskos, C.M. Yip and J.L. Brash, "Effects of heat/citric acid reprocessing on high flux polysulfone dialysers", ASAIO Journal, 48, 45-56 (2002).

R.M. Cornelius, J.G. Archambault, L. Berry, A.K.C. Chan and J.L. Brash, "Adsorption of proteins from infant and adult plasma to biomaterial surfaces", J. of Biomedical Mat. Res., 60, 622-632 (2002).

### Refereed Conference Proceedings

W.G. McClung, D.E. Babcock, and J.L. Brash, "Platelet adhesion to a plasminogen-specific surface (lysine-derivatized polyethylene) from whole blood". 7th World Biomaterials Congress, Sydney, 1714 (2004).

J.L. Brash, R.M. Cornelius, A.P. Hitchcock, T. Araki C. Morin, A. Scholl, A. Doran "Soft X-ray spectromicroscopy of fibrinogen on polystyrene: poly(methyl methacrylate) polymer blend surfaces". 7th World Biomaterials Congress, Sydney, 1637 (2004).

J.L. Brash, R.M. Cornelius, R. Denk, M. Grunze "Adsorption of Plasma Proteins to a Platelet Resistant Polyphosphazene (Polyzene<sup>®</sup>-F)". 7th World Biomaterials Congress, Sydney, 298 (2004).

T.M. Massa, J.L.Brash, J.P. Santerre, "Biological Mapping of Fluorinated Surface Modifier Function on a Polyetherurethane". 7th World Biomaterials Congress, Sydney, 299 (2004).

L.D. Unsworth, Z.Tun, H. Sheardown, J. L.Brash., "Structural evolution of end-tethered PEO layers chemisorbed on gold studied by specular neutron reflectometry: effects on protein repulsion." 7th World Biomaterials Congress, Sydney, 1636 (2004).

### **BROOK, Michael A. (Associate Member, Professor, Department of Chemistry)**

**Research Interests:** Organosilicon chemistry, silicon synthesis, biocompatible silica, silicon-biopolymer interactions.



### Professional Organizations

Regional Editor, The Americas

Member:

- American Chemical Society
- Chemical Institute of Canada
- Silicon Chemistry (a journal)

### Papers in Refereed Journals

R.J. Hodgson, M.A. Brook and J.D. Brennan, "Capillary-Scale Monolithic Immunoaffinity Columns for Immunoextraction with In-Line Laser-Induced Fluorescence Detection". Anal.Chem. In press 2005.

H. Dong, M.A. Brook and J.D. Brennan, "A New Route to Monolithic Methylsilsesquioxanes: Gelatin Behavior of Methyltrimethoxysilane and Morphology of Resulting Methylsilsesquioxanes under One-Step and Two-Step Processing", Chem. Materials 17, 2807-2816 (2005).

- S. Balduzzi, M.A. Brook and M.J. McGlinchey, "Diastereoselective Addition of Allyl- and Crotylstannanes to Dicobalt-Complexed Acetylenic Aldehyde", *Organometallics*, 24, 2617-2627 (2005).
- P. Kovarik, R.J. Hodgson, T. Covey, M.A. Brook and J.D. Brennan, "Capillary-Scale Frontal Affinity Chromatography/MALDI Tandem Mass Spectrometry Using Protein-Doped Monolithic Silica Columns", *Anal. Chem.* 77, 3340-3350 (2005).
- A. Masaaki, J. Schinkel, M.A. Brook, M.J. McGlinchey and J.F. Britten, "Rac/meso Transformations of Disiloxane-bis(1-indenyl)-ansa-ferrocenes: An x-ray crystallographic and NMR Study", *Organometallics*, 24, 1533-1543 (2005).
- S. Xihua, J.A. Cruz-Aguado, Y. Chen, Z. Zhang, M.A. Brook and J.D. Brennan, "Properties of Human Serum Albumin Entrapped in Sol-Gel-Derived Silica Bearing Covalently Tethered Sugars", *Chem. Mater.* 17, 1174-1182 (2005).
- H. Chen, Y. Chen, H. Sheardown, M.A. Brook, Immobilization of heparin on a silicone surface through a PEG spacer. *Biomaterials*. In press 2005.
- H. Chen, Z. Zhang, Y. Chen, M.A. Brook, H. Sheardown, Protein repellent silicone surfaces by covalent immobilization of poly (ethylene oxide). *Biomaterials*. 26: 2391-2399 (2005).
- H. Chen, M.A. Brook, Y. Chen, and H. Sheardown, Surface properties of PEO silicone composites: controlling protein adsorption. *J Biomater Sci Polym Edn* 16: 531-548 (2005).
- A. Ragheb, M.A. Brook and M. Hrynyk, "Highly active, lipase silicone composites", *Biomaterials* 26, 1653-1664 (2005).
- A. Masaaki, J. Schinkel, L. Freiburger and M.A. Brook, "Silicone compatible, Siloxane-Supported Organometallic Compounds and their catalytic activities for the Hydrosilylation of Vinylsilanes and Dienes", *J. Chem. Soc., Dalton Trans.*, 74-81 (2005).
- L. Muxin, E. Pacard, A.M. Ragheb, P.M. Zelisko and M.A. Brook, "Stabilisation of Protein-Containing Water-in-Oil Emulsions", *Cahiers de Formulation*, 11, 152-162 (2004).
- D. Tleugabulova, A.M. Duft, Z. Zhang, Y. Chen, M.A. Brook and J.D. Brennan, "Evaluating Growth mechanisms of Silica Particles Using Fluorescence Anisotropy Decay Analysis", *Langmuir* 20(14), 5924-5932 (2004).
- J.A. Cruz-Aguado, Y. Chen, Z. Zhang, M.A. Brook and J.D. Brennan, "Entrapment of Src protein Tyrosine Kinase in Sugar-Modified Silica", *Anal. Chem* 76 (14), 4182-4188 (2004).
- D. Tleugabulova, A.M. Duft, Z. Zhang, Y. Chen, M.A. Brook, and J.D. Brennan, "Evaluating Formation and Growth Mechanisms of Silica Particles using Fluorescence Anisotropy Decay Analysis", *Langmuir*, 20 (14) 5924-5932 (2004).
- J.A. Cruz-Aguado, Y. Chen, Z. Zhang, N.H. Elowe, M.A. Brook and J.D. Brennan, "Ultrasensitive ATP Detection Using Firefly Luciferase Entrapped in Sugar-Modified Sol-Gel Derived Silica", *J. Am. Chem. Soc.*, 126, 6878-6879 (2004)
- R.J. Hodgson, Y. Chen, Z. Zhang, D. Tleugabulova, H. Long, X. Zhao, M. Organ, M.A. Brook and J.D. Brennan, "Protein-Doped Monolithic Silica Columns for Capillary Liquid Chromatography Prepared by the Sol-Gel Method: Applications to Frontal Affinity Chromatography", *Anal. Chem.* 76, 2780-2790 (2004).
- A. Ragheb, H. Chen, M.L. Marshall, M. Hrynyk, H. Sheardown and M.A. Brook, "Controlling Protein Deposition at Silicone Elastomer Interfaces", *Polym. Prep. (Amer. Chem. Soc., Div. Polym. Chem.)*, 45(1), 602-603 (2004).
- P.M. Zelisko, J.J. Coe-Ranger and M.A. Brook, "The Interaction of Proteins with Functionalized Silicones", *Polym. Prep. (Amer. Chem. Soc., Div. Polym. Chem.)* 45(1), 604-605 (2004).
- J.J. Coe-Ranger, P.M. Zelisko, M.A. Brook, "Ionic Silicone Surfactants in Water-in-Silicone Oil Emulsions Containing proteins", *Polym. Prep. (Amer. Chem. Soc., Div. Polym. Chem.)* 45(1), 674-675 (2004).
- L. Liang, J.M. Dickson, J. Jiang, and M.A. Brook, "Effect of Low Flow Rate on pervaporation of 1, 2-dichloroethane with Novel Polydimethylsiloxane Composite Membranes", *J. Membrane Sci.*, 231 (1-2), 71-79 (2004).
- M.A. Brook, Y. Chen, K. Guo, Z. Zhang and J.D. Brennan, "Sugar-Modified Silanes: Precursors for Silica Monoliths", *J. Mater. Chem.*, 14, 1469-1479 (2004).

D. Tleugabulova, Z. Zhang, Y. Chen, M.A. Brook and J.D. Brennan, "Fluorescence Anisotropy in Studies of Solute Interactions with Covalently Modified Colloidal Silica Nanoparticles", *Langmuir*, 20, 848-854 (2004).

M.A. Brook, H. Chen and H. Sheardown, "Silicone Elastomers for reduced protein adsorption", *Biomaterials*, 25, 2273-2282 (2004).

A. Ragheb, M.A. Brook and M. Hrynyk, "Highly Activated Silicone Entrapped Lipase", *Chem. Commun.*, 2314-2315 (2003).

T.R. Besanger, Y. Chen, A.K. Deisingh, R. Hodgson, W. Jin, S. Mayer, M.A. Brook and J.D. Brennan, "Screening of Inhibitors Using Enzymes Entrapped in Sol-Gel Derived Materials", *Anal. Chem.*, 75, 2382-2391 (2003).

G. Hu, F. LaRonde and M.A. Brook, "Amino Acid-Terminated Silicone", *Chemistry*, 1, 99-1065, (2002)

P. Zelisko, M. A. Brook "Stabilization of  $\alpha$ -Chymotrypsin and Lysozyme Entrapped in Water-In-Silicone Oil Emulsions, *Langmuir* 18, 8982, (2002)

M. Mohamed, M.A. Brook, Allylsilane-Modified Amino Acids from the Claisen Rearrangement. *Helv. Chim. Acta*, 85, 4165 (2002).

C Paul M. Zelisko, and M.A. Brook, "Modified silicones for the stabilisation of proteins and enzymes in emulsions: Potential Vaccine Delivery Systems", *Polym. Prep. (Am. Chem. Soc., Div. Polym. Chem.)*, 42(2), 115-116 (2001).

F Gilles Sèbe and M.A. Brook, "Hydrophobization of Wood Surfaces: Covalent Grafting of Silicone Polymers", *Wood Sci. Tech.*, 35, 269-282 (2001).

M.A. Brook and P. Zelisko "Exploiting Silicone-Protein Interactions: Stabilization Against Denaturation At Interfaces", *Polym. Prep. (Am. Chem. Soc., Div. Polym. Chem.)*, 42(1), 97-98 (2001).

C Mohamed, M.A. Brook, "Synthesis of Allylsilane-Containing Amino Acids via the Claisen Rearrangement", *Tetrahedron Lett.*, 42, 191-193 (2001).

## Current Research Projects

### ***PROTEIN-DOPED BIOCOMPATIBLE SILICA FOR HIGH THROUGHPUT DRUG SCREENING***

Controlled synthesis of silica; surface modification; enzyme kinetics. Scientific challenges; understanding interfacial interactions with proteins.

### ***SILICONE BIOMATERIALS FOR THE EYE, CORNEA AND LENSES***

Silicone preparation, surface modification, protein and cell adsorption: Scientific challenges; understanding how to make silicone look like ocular tissue.

### ***FUNCTIONAL SURFACTANTS FOR PROTEIN CLEANING***

Silicone preparation, colloid/surface characterization, protein stabilization.

### ***BIOACTIVE PAPER: BINDING TiO<sub>2</sub> TO PAPER***

Microparticle synthesis, particle surface adhesion, paper photochemistry, bacterial disinfection.

**DALNOKI-VERESS, Kari (Associate Member, Associate Professor, Department of Physics and Astronomy)**

**Research Interests:** Soft Condensed matter, Polymer Physics, Bio-Physics



**Professional Organizations:**

Member:

- American Physical Society
- Canadian Association of Physicists
- Materials Research Society

**Papers in Refereed Journals**

B. Frick, C. Alba-Simionesco, G. Dosseh, C. LeQuellec, A.J. Moreno, J. Colmenero, A. Schonhals, R. Zorn, K. Chrissopoulou, S.H. Anastasiadis, K. Dalnoki-Veress, "Inelastic neutron scattering for investigating the dynamics of confined glass forming liquids", *J. Non-cryst. Solids*, in press.

M.V. Massa, M.S.M. Lee and K. Dalnoki-Veress, "Crystal nucleation of polymers confined to droplets: Memory effects", *J. Polym. Sci. Part B: Polym. Phys.*, (2005).

L. Si, M.V. Massa, K. Dalnoki-Veress, H.R. Brown and R.A.L. Jones, "Shear deformation in thin free-standing polymer films as a probe of entanglement in confined systems", *Phys. Rev. Lett.*, 94, 127801 (2005).

M.V. Massa and K. Dalnoki-Veress, "Homogeneous crystallisation of poly(ethylene oxide) confined to droplets: the dependence of the crystal nucleation

rate on length-scale and temperature", *Phys. Rev. Lett.*, 29, 255509 (2004).

C. Lu, R. Richardson, R. Pelton, T. Cosgrove, S. Satija and K. Dalnoki-Veress, "PEO Penetration into Water-plasticized Poly(vinyl phenol) thin Films", *Macromolecules*, 37, 494 (2004).

M. V. Massa, K. Dalnoki-Veress, J. A. Forrest, "Crystallization Kinetics and Crystal Morphology in Thin Poly(ethylene oxide) Films", *European Phys. J.E.* 11, 191 (2003)

B. Frick, K. Dalnoki-Veress, J. A. Forrest, J. Dutcher, and C. Murray, and A. Higgins, "First inelastic neutron scattering studies on thin free standing polymer films", *European Phys. J. E.* 12, 195, (2003).

K. Dalnoki-Veress, J.R. Dutcher and J.A. Forrest, "Dynamics and Pattern Formation in Thin Polymer Films", *Physics in Canada*, March (2003).

M.V. Massa, J.L. Carvalho, and K. Dalnoki-Veress, "Direct visualisation of homogeneous and heterogeneous crystallisation in an ensemble of confined domains of poly(ethylene oxide)", *European Phys. J. E.*, 12, 111 (2003).

C. Roth, B.G. Nickel, J.R. Dutcher and K. Dalnoki-Veress, "Differential Pressure Experiment to Probe the Onset of Hole Formation in Freely-Standing Polystyrene Films", *Rev. Sci. Inst.*, 74, 2796 (2003).

J.A. Forrest and K. Dalnoki-Veress, "The Glass Transition in Thin Polymer Films", *Advances in Colloid and Interface Science*, 94, 167-195 (2001).

C. Gigault, K. Dalnoki-Veress and J.R. Dutcher, "Changes in the Morphology of Self-Assembled Polystyrene Microsphere Monolayers Produced By Annealing", *J. Colloid Inter. Sci.* 243, 143-155 (2001).

K. Dalnoki-Veress, J.A. Forrest, C. Murray, C. Gigault, and J.R. Dutcher, "Molecular Weight Dependence of Reductions in the Glass Transition Temperature of Thin Freely Standing Polymer Films", *Phys. Rev. E.* 63, 031801-1 - 031801-10 (2001).

**Refereed Conference Proceedings:**

J.A. Forrest and K. Dalnoki-Veress, "Sub-Glass Transition Interface Formation Between an Immiscible Glass Rubber Pair", *J. Polym. Sci. Part B: Polym. Phys.*, 39, 2664-2670, (2001).

K. Dalnoki-Veress, J.A. Forrest, M.V. Massa, A. Pratt and A. Williams, "Crystal Growth Rate in

Ultrathin Films of Poly(ethylene oxide)", J. Polym. Sci. Part B: Polym. Phys., 39, 2615-2621, (2001).

K. Dalnoki-Veress, B. Frick, J. Forrest, J.R. Dutcher, C. Murray and A. Higgins, "First Inelastic Neutron Scattering Studies on Thin Free Standing Polymer Films", Institut Laue-Langevin (ILL) Millenium Symposium Technical Report (2001).

## Current Research Projects

### POLYMERS AT SURFACES AND INTERFACES

*K. Dalnoki-Veress*

*In the McMaster Polymer Physics Laboratory, we study polymeric materials, which are ubiquitous in their use, from basic plastic components and packaging materials, to drug delivery and display technologies. These systems do not necessarily exhibit the same properties as bulk materials. Thin films provide a convenient sample geometry in which to study confinement effects in order to answer the fundamental question: what happens to macromolecules when they are confined into a space smaller than what the molecule would occupy in the bulk? We address these questions with several tools, scanning probe microscopy, optical microscopy, dynamic light scattering, ellipsometry, as well as some unique home-built experiments. Our efforts can be summarised under three broad and overlapping areas. First of all we study surface energy and mechanical properties of thin films and have designed a new tool to achieve this goal. Careful measurement will allow us to further our understanding of an area that is still theoretically poorly understood and remains experimentally very challenging. In our second focus area we are interested morphologies which 'self-assemble'. We first of all try to understand why these morphologies appear, for example: what basic physics underlies the observed morphology? Once the physics governing the morphologies is understood, we can perhaps control aspects of the morphology so that potentially useful structures may be made. Our third main area of interest deals with dynamics and crystallisation of in confined spaces. While some of our projects are expected to result in improvements to existing technologies, our primary, long term goal is to obtain a more general understanding of the effects of confinement, surfaces, and interfaces in soft material systems.*

## DICKSON, JAMES M. (Professor)

**Research Interests:** transfer phenomena in membranes, reverse osmosis, ultrafiltration, electro dialysis, novel polymers.



## Professional Organizations

Member:

- Canadian Society for Chemical Engineering
- American Institute of Chemical Engineers
- North American Membrane Society

## Papers in Refereed Journals

J. Garcia-Aleman, J.M. Dickson, and A.M. Mika, "Experimental Analysis Modeling, and Theoretical Design of McMdaster Pore-filled Nanofiltration Membranes", J. Membr. Sci., 240, 237-255 (2004).

J. Garcia-Aleman and J.M. Dickson, "Permeation of Mixed-salt Solutions with Commercial and Pore-filled Nanofiltration Membranes: Membrane Charge Inversion Phenomena", J. Membr. Sci., 239, 163-172 (2004).

W. Jiang, R. F. Childs, A. M. Mika, J. M. Dickson "Pore-filled cation-exchange membranes containing poly(styrenesulfonic acid)gels", Desalination, 159, 253-266, (2003).

J. Garcia-Aleman, J. M. Dickson "Mathematical modeling of nanofiltration membranes with mixed electrolyte solutions" J. Membr. Sci., 235, 1-13 (2004).

R.F. Childs, J. Weng, M. Kim and J.M. Dickson, "Formation of pore-filled microfiltration membranes using a combination of modified interfacial polymerization and grafting", J. Polym. Sci, A. Polym Chem 40, 242-250 (2002).

A.M. Mika, R.F. Childs and J.M. Dickson, "Salt separation and hydrodynamic permeability of porous membranes filled with pH sensitive gel", J. Membrane Science, 206, 19-30 (2002).

D.R. Woods, D. Kourti, P.E. Wood, H. Sheardown, C.M. Crowe, and J.M. Dickson, "Assessing problem solving skills. Part 2: Assessing the process of problem solving", Chem. Eng. Ed., 36(1), 60-67 (2002).

R.F. Childs, A.M. Mika, A.K. Pandey, C. McCrory, S. Mouton and J.M. Dickson, "Nanofiltration using pore-filled membranes: effect of polyelectrolyte composition on performance", Separation and Purification Technology, 22-23, 507-517 (2001).

A.K. Pandey, R.F. Childs, M. West, J.N.A. Lott, B.E. McCarry and J.M. Dickson, "Formation of pore-filled ion-exchange membranes using in-situ cross-linking: Poly(vinylbenzyl ammonium salt) filled membranes", J. Polym. Sci. Part A: Polym. Chem., 39, 807-820 (2001).

## Patents

A.M. Mika, R.F. Childs and J.M. Dickson, "Microporous membranes and uses thereof", McMaster University, filed PCT, October 1996, issued USA Patent 6,258,276, July 10, 2001, PCT awarded Australia, New Zealand, Singapore, 2002.

R.F. Childs, J.M. Dickson, D.R. Gagnon, K. Rilling, "Membrane preparation from porous substrates by interfacial polymerization in pores, preferably containing photochemically active groups for further derivatization", US Patent 5,627,217, May 6, 1997 and a European Patent in 2002.

## FILIPE, CARLOS D.M. (Assistant Professor)

**Research Interests:** environmental biotechnology, wastewater treatment, metabolic modelling, membrane bioreactors.



## Professional Organizations

Member:

- Water Environment Federation
- Water Environment Association of Ontario
- American Society for Microbiology
- Association of Environmental Engineering and Science Professors

## Papers in Refereed Journals

D.M Kanani, R. Ghosh and C.D.M. Filipe  
Manipulation of protein-protein separation by ultrafiltration using a facilitating agent.  
Biotechnology and Bioengineering (2003)

R. Childs, A. Mika, C.D.M. Filipe and R. Ghosh.  
Supported structured Gel Based Membranes with Environmentally Responsive Pore-sizes and their use in Size-Based Separation of Molecules and/or Particles. Provisional U.S. Patent Application was filed.

C.D.M. Filipe, G.T. Daigger and C.P.L. Grady Jr.,  
"pH as a key factor in the competition between glycogen accumulating and phosphorus accumulating organisms", Water Environment Research, 73, 223-232 (2001).

phosphate accumulating and glycogen accumulating organisms”, Water Environment Research, 73, 213-222 (2001).

C.D.M. Filipe, G.T. Daigger and C.P.L. Grady jr., “Stoichiometry and kinetics of acetate uptake under anaerobic conditions by an enriched culture of phosphorus accumulating organisms at different pHs”, biotechnology and Bioengineering, 76, 32-43 (2001).

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C.D.M. Filipe, J. Meinhold, S. Jørgensen, G.T. Daigger, C.P.L. Grady Jr, “The effects of equalization on biological phosphorus removal processes”, Water Environment Research, 73, 276-294 (2001).

### **Refereed Conference Proceedings**

C.D.M. Filipe, G.T. Daigger, C.P.L. Grady Jr., “An integrated metabolic model for the anaerobic and aerobic metabolism of glycogen accumulating organisms”, Third IWA International Specialized Conference on Microorganisms in activated Sludge and Biofilm Processes, Rome (2001).

C.D.M. Filipe, G.V. Crawford, B. Johnson, and G.T. Daigger, “Integrating ASM2d models into whole plant mass balance simulators”, Proceedings of the 30<sup>th</sup> Western Ontario Water Association Technical Symposium and OPCEA Exposition, Toronto, ON (2001).

T. Constantine, C.D.M. Filipe, M.D. Elliott, G.V. Crawford, G.T. Daigger, “New process configuration to achieve year round nitrification at low SRTs”, Proceedings of the 30<sup>th</sup> Western Ontario Water Association Technical Symposium and OPCEA Exposition, Toronto, ON (2001).

G.V. Crawford, C.D.M. Filipe, S. Black, “Enhanced primary treatment for sewage, SSOs and CSOs. Proceedings of the 30<sup>th</sup> Western Ontario Water Association Technical Symposium and OPCEA Exposition, Toronto, ON (2001).

### **GHOSH, RAJA (Assistant Professor)**

**Research Interests:** bioseparation using ultrafiltration, bioseparation using membrane chromatography, biomimetic membranes.



### **Professional Organizations**

Member:

- American Institute of Chemical Engineers

### **Papers in Refereed Journals**

R. Ghosh, Membrane chromatographic immunoassay method for rapid quantitative analysis of specific sesum antibodies. Biotechnology and Bioengineering (accepted)

R. Ghosh, Enhancement of membrane permeability by gas-sparging in submerged hollow-fibre ultrafiltration of macromolecular solutions: role of module design. Journal of Membrane Science (accepted)

C.D.M. Filipe and R. Ghosh, Effects of protein-protein interaction in ultrafiltration based fractionation processes, Biotechnology and Bioengineering (in press).

R. Ghosh, Fractionation of human plasma proteins by hydrophobic interaction membrane chromatography, *Journal of Membrane Science*, Vol 260, 112 (2005).

Y. Wan, R. Ghosh, G. Hale and Z.F. Cui, Fractionation of bovine serum albumin and monoclonal antibody Alemtuzumab using carrier phase ultrafiltration, *Biotechnology and Bioengineering*, Vol 90, 303 (2005).

Y. Wan, S.S. Vasani, R. Ghosh, G. Hale and Z.F. Cui, Separation of monoclonal antibody Alemtuzumab monomer and dimers using ultrafiltration, *Biotechnology and Bioengineering* Vol 90, 422 (2005).

R. Ghosh, Separation of human albumin and IgG by a membrane-based integrated bioseparation technique involving simultaneous precipitation, microfiltration and membrane adsorption, *Journal of Membrane Science*, vol. 237 109 (2004).

D. Kanani, R. Ghosh and C.D.M. Filipe, A novel approach for high-resolution protein-protein separation by ultrafiltration using a dual-facilitating agent, *Journal of Membrane Science*, vol. 243 223 (2004).

Y. Wan, R. Ghosh and Z.F. Cui, Separation of human serum albumin and human immunoglobulins using carrier phase ultrafiltration, *Biotechnology Progress*, vol. 20 1103 (2004).

R. Ghosh, "Separation of human albumin and IgG by a membrane-based integrated bio-separation technique involving simultaneous precipitation, microfiltration and membrane adsorption", *Journal of Membrane Science*, 237, 109-117 (2004)

R. Ghosh, Novel Cascade ultrafiltration configuration for continuous, high-resolution protein-protein fractionation: a simulation study, *Journal Membrane Science*, 226, p. 673-682 (2003)

R. Ghosh, Y. Wan, Z.F. Cui and G. Hale, "Parameter scanning ultrafiltration: rapid optimisation of protein separation", *Biotechnology and Bioengineering* 81, 673 (2003).

R. Ghosh, "Purification of lysozyme by microporous PVDF membrane based chromatographic process", *Biochemical Engineering Journal*, 14, 109 (2003)

R. Ghosh, "Study of membrane fouling by BSA using pulsed injection technique", *Journal of Membrane Science* 195, 117 (2002).

R. Ghosh, "Protein separation using membrane chromatography: opportunities and challenges" (invited review article) *Journal of Chromatography A* 952, 13 (2002).

V. Seshadri, R. Ghosh and Z.F. Cui, "Design of cone-and-plate test cell for ultrafiltration", *Desalination*, 146, 219 (2002).

Y. Wan, R. Ghosh and Z.F. Cui, "High-resolution ultrafiltration processes for protein fractionation", *Desalination*, 144, 301 (2002).

R. Ghosh, "Fractionation of biological macromolecules using carrier phase ultrafiltration", *Biotechnology and Bioengineering* 74, 1-11 (2001).

R. Ghosh, "Bioseparation using supported liquid membrane chromatography", *Journal of Membrane Science*, 192, 243-247 (2001).

R. Ghosh, "Separation of proteins using hydrophobic interaction membrane chromatography", *Journal of Chromatography A* 923, 59-64 (2001).

R. Ghosh, "Novel membranes for simulating biological barrier transport", *Journal of Membrane Science*, 192, 145-154 (2001).

## Books

R. Ghosh, "Protein Bioseparation Using Ultrafiltration: Theory, Applications and New Developments" ISBN 1-86094-317-9), Imperial College Press/World Scientific Publishing Pte Ltd. (2003).

## Chapters In Books

R. Ghosh, "Protein bioseparation using membrane adsorbents: combining high-resolution with high-throughput, in *Protein Production, Aggregation and Degradation in Recombinant Bacterial Factories* (editor: A. Villaverde), Research Signpost (2002).

**HAMIELEC, ARCHIE (Emeritus Professor)**

**Research Interests:** polymer production technology, kinetics, reactors, characterization.



**Professional Organizations**

Member:

- American Institute of Chemical Engineers
- Canadian Society for Chemical Engineering
- Fellow, Chemical Institute of Canada
- Fellow, Royal Society of Canada

**Papers in Refereed Journals**

E. Kolodka, W.-J. Wang, S. Zhu and A.E. Hamielec, “Molecular weight dependence on domain formatin of grafted poly(ethylene-co-propylene) in polypropylene matrix”, *Macromol. Rapid Commun.*, 23, 470-473 (2002).

E. Kokko, W.-J. Wang, J.V. Seppala and S. Zhu, “Structural analysis of dimethylsilylbis(indenyl)zirconium dichloride/methylaluminoxane catalyzed polyethylene”, *J. Polym. Sci., Polym. Chem.*, 40, 3292-3301 (2002).

J.B.P. Soares and A.E. Hamielec, “Polymer reactor principles: Polyolefins”. 1<sup>st</sup> North American Symposium on Chemical Reaction Engineering, Houston, Texas, U.S.A., January 6-9 (2001).

E. Kolodka, W.-J. Wang, P.A. Charpentier, S. Zhu and A.E. Hamielec, “Long chain branching in Ethylene Polymerization using Zirconocene Catalysts”, *Polymer*, 41, 3985-3991 (2000).

**HRYMAK, ANDREW N. (Professor, Chair)**

**Research Interests:** polymer processing, reactive extrusion and molding, process analysis, design and optimization.



**Professional Organizations**

Member:

- Canadian Society for Chemical Engineering
- American Institute of Chemical Engineers
- Polymer Processing Society
- Society of Plastics Engineers
- Society of Rheology
- Professional Engineers of Ontario

**Papers in Refereed Journals**

V. L. Bravo, A. N. Hrymak, J.D. Wright. “Study of particle trajectories, residence time and flow behavior in kneading discs of intermeshing co-rotating twin scw extruders”, *Poly. Eng. Sci.* 44, 779-793 (2004).

L. Gu, S. Zhu, A.N. Hrymak, "Acidic and Basic Hydrolysis of poly(N-vinylformamide)", J. Appl. Polym. Sci, 86, 3412-3419 (2002).

L. Gu, S. Zhu, A.N. Hrymak, "Synthesis and flocculation performance of graft copolymer of N-vinylformamide and poly(dimethylaminoethylmethacrylate) methyl chloride macromonomer", Colloid Polym Sci, 280, 167-175 (2002).

H.J. Larrazabal, A.N. Hrymak "Flow instabilities of linear PE in Capillary Dies – materials of construction of dies", Int Polym Proc., 17, 44-48, (2002).

J. Wang, A.N. Hrymak, and R.H. Pelton, "Compactable porous and fibrous beds formed from dilute pulp suspensions", Industrial & Engineering Chemistry Research, 41(3), 572-578 (2002).

J. Wang, A.N. Hrymak, and R.H. Pelton, "Specific Surface and Effective Volume of Water Swollen Pulp Fibers by a Permeability Method", J. Pulp Paper Science, 28(1) 13-16 (2002).

J. Wang, R.H. Pelton, A.N. Hrymak and Y. Kwon, "New insights into dispersed air effects in brownstock washing", Tappi, 84 (1), 101 (2001).

M. Rodic and A.N. Hrymak, "The modified imbedded disk retraction method for measurement of interfacial tension in polymer melts", submitted to Rheologica Acta, 40, 339-348, (2001).

L. Gu, S. Zhu, A.N. Hrymak, R.H. Pelton "Nature of Poly(N-vinylformamide) Gel Formed in Free Radical Polymerization of N-vinylformamide", Macromol. Rapid Commun., 22, 212-214, (2001).

L. Gu, S. Zhu, A.N. Hrymak, R.H. Pelton "Kinetics and Modelling of Free Radical Polymerization of N-Vinylformamide", Polymer, 42, 3077-3086, (2001).

L. Gu, S. Zhu, A.N. Hrymak, and R.H. Pelton, "The Nature of Crosslinking in Nvinylformamide Free Radical Polymerization, Macromol". Rapid Commun., 22, 212 (2001).

## **JONES, KIM S. (Assistant Professor)**

**Research Interests:** Tissue engineering, regenerative medicine, immune and inflammatory responses to biomaterials



### **Professional Organizations**

Member:

- Canadian Society of Biomaterials
- Canadian Society for Chemical Engineering

### **Papers in Refereed Journals**

K.S. Jones, R.M. Gorczynski, M.V. Sefton, "In vivo recognition by the host adaptive immune system of microencapsulated xenogeneic cells", Transplantation, 78(1), 1454-1462 (2004).

### **Patents**

McKersie, B.D., Bowley, S.R. Jones, K.S., Samis, K. Enhanced Storage Organ Production in Plants. Patent # 6,518,486 - Awarded February 11, 2003

### **Chapters in Books**

McKersie, B.D., Bowley, S.R., Jones, K.S., Gossen, B. (1999) Winter survival of transgenic Medicago sativa over-expressing superoxide dismutase. In M.F. Smallwood, Calvert, C.M. and Bowles (eds.) Plant Responses to Environmental Stress, Bios Scientific Publishers.

## **LOUTFY, RAFIK (Professor)**

**Research Interests:** Entrepreneurship, Innovation, knowledge management, alternate energy sources, solar cells, photovoltaic engineering.



### **Professional Organizations**

- Board of Editors Member Research and Technology Management Journal

### **Papers in Refereed Journals**

“Molecular Structure and photoactivity in perylene tetracarboxylic diimides”, J. M. Duff, A.M. Hor, R.O. Loutfy and A.R. Melnyk, Proc. 2nd Int. Symp. on Chemistry of Functional Dyes, Vol. 2, 564 (1993) Ed. Z. Yoshida and Y. Shirota, MITA press.

Management of Innovation in Large Corporation – Xerox Experience” R.O. Loutfy and L. Belkhir; Research & Technology Journal, in press 2001

### **Patents**

43 US, Canadian & European Patents from 1979 to 2000. The latest three are listed:

**US Patent 6,124,409** “Processes for preparing copolymers” T. H. Ng, H.K. Mahabadi, M.C. Tam, G. Kovacs, E.M. Peters, R.O. Loutfy; September 26, 2000.

**Canadian Patent 2,077,294** “Infrared or red light sensitive migration imaging member” M.C. Tam, J.P. Meester, H.M. Aboushaka, R.O. Loutfy, G.J. Kovacs, G.J. Jennings January 17, 1994

**US Patent 5,728,747** “Stable Free Radical Polymerization Processes and Compositions Thereof” P.M. Kazmaier; B.K. Keoshkerian; R.O. Loutfy; K.A. Moffat; M.K. Georges; G.K. Hamer; R.P.N. Veregin, Mar. 17, 1998

## **KEVLAHAN, Nicholas K.-R. (Associate Member, Associate Professor, Department of Mathematics & Statistics)**

**Research Interests:** Turbulence, wavelets, numerical simulation, fluid dynamics.



### **Professional Organizations**

Member:

- Canadian Mathematics Society
- Canadian Applied and Industrial Mathematics Society
- Marie Curie Fellowship Society

## Papers in Refereed Journals

N.K-R. Kevlahan, Stochastic differential equation models of vortex merging and reconnection. To appear in Phys. Fluids. (2005).

N.K-R. Kevlahan and J. Wadsley, Suppression of three-dimensional flow instabilities in tube bundles. To appear in J. Fluids Strucs. (2005).

N.K-R. Kevlahan and O.V. Vasilyev, An adaptive wavelet collection method for fluid-structure interaction at high Reynolds numbers. To appear in SIAM J. Sci. Comput. (2005).

O.V. Vasilyev and N.K-R. Kevlahan, An adaptive multilevel wavelet collocation method for elliptic problems. J. Comp. Phys. 206, 412-431 (2005).

O.V. Vasilyev and N.K-R. Kevlahan, . Hybrid wavelet collocation-Brinkman penalization method for complex geometry flows. Int. J. Num. Meth. Fluids 30, 531-538, (2002).

B. Dubrulle, J.-P. Laval, S. Nazarenko, and N.K-R. Kevlahan. Derivation of equilibrium profiles in plane parallel flows from a dynamical subgrid model. Phys. Fluids 13, 2045-2064, (2001).

N.K-R. Kevlahan and J.-M Ghidaglia. Computation of turbulent flow past an array of cylinders using a spectral method with Brinkman penalization. Eur. J. Mech. B 20, 333-350, (2001).

## Current Research Projects

***NO***

### ***NLINEAR RDT THEORY OF NEAR-WALL TURBULENCE***

*S. Nazarenko, N.K.-R. Kevlahan, and B. Dubrulle. (2000).*

*It was shown that the celebrated log law of the wall exists as an exact analytical solution of a WKB Rapid Distortion Theory approximation to the Navier-Stokes equations if the initial turbulence vorticity (debris of the near-wall vortices penetrating into the outer regions) is statistically homogeneous in space and shortly correlated in time. The main contribution to the shear stress comes from very small turbulent scales which are close to the viscous cut-off and which are elongated in the stream-wise direction (streaks). This is the first paper to calculate mean turbulent velocity profiles near a wall directly from the dynamical equations, rather than using scaling hypotheses.*

### ***ADAPTIVE WAVELET METHOD FOR FLUID-STRUCTURE INTERACTION***

*N. K-R. Kevlahan*

*In recent research with Oleg Vasilyev, I have been developing an efficient adaptive wavelet method for incompressible fluid-structure interaction in two dimensions. Because this code is based on the Navier-Stokes equations written in terms of primitive variables, it is relatively straightforward to extend it to three dimensions and to compressible flow. Since the fast wavelet transform has complexity  $O(N)$  (where  $N$  is the number of active grid points), it should scale well for large problems. The development and testing of the parallel code will take advantage of the sharcnet network of parallel computers.*

**KOURTI, THEODORA (Adjunct,  
Associate Professor)**

**Research Interests:** Statistical methods for data mining, process analysis, monitoring and fault diagnosis. Process Analytical Technology, Bioinformatics.

**Professional Organizations**

Member:

- American Institute of Chemical Engineers
- Canadian Society of Chemical Engineers, Chemical Institute of Canada
- Technical Chamber of Greece (Greek Professional Engineers)
- International Chemometrics Society
- Archeological Institute of America
- Hellenic Canadian Academic Association Ontario (Secretary)

**Refereed Journal Papers (Selected)**

S. Garcia Munos, J.F. MacGregor, T. Kourti “Product Transfer between sites using joint Y\_PLS”. Chemometrics and Intelligent Laboratory Systems in press (2005).

T. Kourti , “Application of Latent Variable Methods to Process control and statistical Process control in Industry”. (special issue of condition monitoring). International Journal of Adaptive control and Signal Processing, 19, 213-246 (2005)

S. Garcia-Munoz, J. F. MacGregor, J.F. Kourti, “Model Predictive monitoring for batch processes with multivariate methods”. Ind. Eng. Chem. Res., 43, 5929-5941 (2004).

T. Kourti, “Abnormal Situation Detection, Three way data and Projection Methods – Robust Data archiving and Modeling for Industrial Applications”. Annual Reviews In Control, 27 (2), 131-138 (2003).

S. Garcia-Munoz, T. Kourti, J. f. MacGregor, A. G. Mateos, G. Murphy. “Troubleshooting of an Industriail Batch Process Using Multivariate Methods”. Ind. Eng. Chem. Res. 42, 3592-3601 (2003).

T. Kourti, “Multivariate Dynamic Data Modelling for Analysis and Statistical Process Control of Batch

Processes, Start–Ups and Grade Transitions”, J. Chemometrics, 17(1), 93-109 (2003).

T. Kourti, “Process Analysis and Abnormal Situation Detection: From Theory to Practice”, IEEE Control Systems, 22(5), 10-25 (2002).

C. Dushesne, T. Kourti, and J.F. MacGregor, “Multivariate SPC for Start ups and Grade Transitions”, AIChE Journal, 48 (12), 2890-2901 (2002).

O. Svensson, T. Kourti, J.F. MacGregor, “A Comparison of Orthogonal Signal Correction Algorithms and Characteristics”, Journal of Chemometrics, 16 pp 176-188 (2002).

D.R. Woods, T. Kourti, P.E. Wood, H. Sheardown, C.M. Crowe, and J.M. Dickson, “Assessing Problem solving skills:1. The context for assessment”, Chemical Engineering Education, American Society for Engineering education Fall 2001 issue.

D.R. Woods, T. Kourti, P.E. Wood, H. Sheardown, C.M. Crowe, and J.M. Dickson, “Assessing Problem solving skills: 2. Assessing the Process of problem solving skills”, Chemical Engineering Education, American Society for Engineering education Winter 2001 issue

**Current Research Projects**

***TOPICS IN MULTIVARIATE ANALYSIS, DATA MINING, ABNORMAL SITUATION DETECTION IN PROCESS INDUSTRIES***

***T. Kourti***

*A variety of projects related to the above topics are available. Multivariate analysis as a tool for analysis and monitoring of processes has originated in this group. There are several theoretical issues to be resolved to extend the applicability of the methods at a wider range of process industries. Multivariate methods as well as other methods, may be applied for data mining in a wide range of applications. Interdisciplinary projects in conjunction with other departments and industry are available. Finally, industrial employees are strongly encouraged to seek a part time Master’s degree where important problems in their own companies (related to data mining and abnormal situation detection) can be addressed as projects in their thesis; similar experience in the past led to very successful interactions, and as a result of the projects, enormous savings for the companies.*

**MacGREGOR, JOHN, F. (University Professor)**

**Research Interests:** multivariate statistical methods for process monitoring and optimisation, polymer reaction engineering.



**Professional Organizations**

Member:

- Association of Professional Engineers of Ontario
- Canadian Institute of Chemical Engineering
- American Institute of Chemical Engineers
- Chemometrics Society of North America

**Papers in Refereed Journals**

J.F. MacGregor, H. Yu, S. Garcia-Munoz and J. Flores-Cerrillo, "Data-base Latent Variable Methods for Process Analysis, Monitoring and Control", *Computers & Chem. Eng.*, Accepted Oct. 2004.

J. Flores-Cerillo and J.F. MacGregor, "Latent variable MPC for Trajectory Tracking in Batch Processes, *J. Process Control*, Accepted, Sept., 2004.

K. Muteki, K., J.F. MacGregor and T. Ueda, "Estimation of Missing Data using Latent Variable Methods with Auxiliary Information", *Chemometrics & Intell. Lab. Systems*, Accepted, Oct., 2004.

P.R.C. Nelson, P.R.C., J.F. Macgregor and P.A. Taylor, "The Impact of Missing Data on PCA and PLS Prediction and Monitoring Applications", *Chemometrics & Intell. Lab. Systems*, Accepted, Sept., 2004.

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## MARLIN, THOMAS E. (Professor)

**Research Interests:** computer process control, real-time plant optimization, optimization of uncertain systems, control structure design.



## Professional Organizations

Member:

- Instrument Society of America
- American Institute of Chemical Engineers

## Papers in Refereed Journals

Y.S. Yip and T.E. Marlin, “The Effect of Model Fidelity on Real-time Operations Optimization”, Comp. Chem. Engr., 28, 267-280 (2004).

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## Chapters in Books

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M. Hough, E. Wood, W.S. Yip and T.E. Marlin, "A WEB Site to Support Active Student Learning in Process Control", Amer. Assoc. of Eng. Ed., Annual Conference, Session 3513, Montreal, Canada, June 16-19, (2002).

T.E. Marlin and D.R. Woods, "Trouble Shooting for CAPE Undergraduate Education", ESCAPE 12, The Hague, Netherlands (2002).

## MHASKAR, PRASHANT (Assistant Professor)

**Research Interests:** Process control, Nonlinear Lyapunov-based and model predictive control, Fault-tolerant control, Control of hybrid systems



## Professional Organizations

- Canadian Society for Chemical Engineering
- American Institute of Chemical Engineers

## Papers in Refereed Journals

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**PELTON, ROBERT H. (Professor, Canada Research Chair in Interfacial Technologies, Principal Investigator: Sentinel)**

**Research Interests:** polymer colloids, water soluble polymers, pulp and paper technology, flocculation, and latex's.



## Professional Organizations

Member:

- Canadian Institute of Chemistry
- Canadian Society for Chemical Engineering
- American Chemical Society
- International Polymer Colloid Group (elected)
- Technical Association of the American Pulp and Paper Industry
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T. Smith-Palmer and R.H. Pelton, "Competitive interactions of dextran sulfate with positively charged particles and polymers", *Colloids and Surfaces A.*, 181, 171-181(2001).

## Current Research Projects

### R.H. Pelton

*I have many projects dealing with the application of colloids, nanoparticles, microgels and surfaces. For a current listing, please see:*

[www.papersci.mcmaster.ca](http://www.papersci.mcmaster.ca)

## SHEARDOWN, HEATHER (Associate Professor)

**Research Interests:** biomaterials, tissue engineering, mathematical modeling of physiologic processes, ophthalmic drug delivery



## Professional Organizations

Member:

- Association of Professional Engineers of Ontario

## Papers in Refereed Journals

H. Chen , Y. Chen, H. Sheardown, M.A. Brook, Immobilization of heparin on a silicone surface through a PEG spacer. *Biomaterials*. In press 2005.

L.D. Unsworth, H. Sheardown, and J.L. Brash, "Polyethylene oxide surfaces of variable chain density by chemisorption of PEO-thiol on gold: Adsorption of proteins from plasma studied by radiolabelling and immunoblotting. *Biomaterials*. In press 2005.

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X. Duan, C.M. Griffith, M.A. Dube and H. Sheardown, "Novel dendrimer based polyurethanes for PEO incorporation", *J. Biomat. Sci. Polym. Edn* 13: 667-690 (2002).

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H. McCormick, R. McMillan, K. Merrett, F. Bensebaa, Y. Deslandes, M.A. Dubé and H. Sheardown, "XPS and water contact angle evaluation of the effect of conditions on peptide chemisorption to gold and silver coated polymer surfaces", *Colloids and Surfaces B: Biointerfaces* 26: 351-363 (2002).

M. Griffith, M. Hakim, S. Shimmura, M.A. Watsky, F. Li, D. Carlsson, M. Nakamura, E. Suuronen, N. Shinozaki, K. Nakata and H. Sheardown, "Artificial corneas: scaffolds for transplantation and host regeneration". *Cornea* 21: S54-61 (2002).

L. Aucoin, C.M. Griffith, G. Plewizier, Y. Deslandes and H. Sheardown, "Interactions of corneal epithelial cells and surfaces modified with cell adhesion peptide combinations" *J. Biomater. Sci. Polym. Edn.* 13: 447-462 (2002).

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A.K. Yeung, J.L. Brash, and H. Sheardown, Controlled delivery of t-PA from a copolymer of HEMA. Society for Biomaterials 2005.

L.A. Wells and H. Sheardown, Fibroblast growth factor delivery for corneal tissue infiltration into porous PDMS scaffold Association for Research in Vision and Ophthalmology 2005.

B.J. Klenkler and H. Sheardown, Epidermal growth factor-modified polydimethylsiloxane for keratoprotheses Association for Research in Vision and Ophthalmology 2005.

M.A. Princz, L. Jones and H. Sheardown, Release of wetting agents from nelfilcon contact lenses. Association for Research in Vision and Ophthalmology. 2005

L. Liu, L. Jones and H. Sheardown, Wetting agent release from contact lenses. Association for Research in Vision and Ophthalmology. 2005.

H. Chen, M.A. Brook and H. Sheardown. "Controlled morphology silicone PEO composites have protein rejecting surfaces". World Biomaterials Congress 2004.

H. Chen, M.A. Brook, and H. Sheardown. "Protein-rejecting silicone Surfaces: Immobilization of PEO by covalent bond". World Biomaterials Congress 2004.

B. Klenkler and H. Sheardown. "Characterization of epidermal growth factor-modified PDMS for artificial corneas". World Biomaterials Congress, 2004.

H. Sheardown and L. W. Jones "In vitro adsorption of albumin and lysozyme from mixed protein solutions to commercial contact lenses". World Biomaterials Congress 2004.

L. Unsworth, Z. Tun, H. Sheardown, J. L. Brash. "Structural evolution of end-tethered PEO layers chemisorbed on gold studied by specular neutron reflectometry: effects on protein repulsion". World Biomaterials Congress 2004.

B. Klenkler and H. Sheardown. "SPR characterization of epidermal growth factor-modified PDMS for artificial corneas" CSCHE 2003.

L. Liu, H. Sheardown. "PDMS/PNIPAAm polymer networks as biomaterials: Glucose permeability, mechanical properties and LCST". CSCHE Conference 2003.

X. Duan and H. Sheardown. "Cross-linking of collagen with dendrimers". CSCHE 2003

H. Chen, M. A. Brook and H. Sheardown "Protein rejecting silicone elastomers". Society for Biomaterials 2003.

L. D. Unsworth, H. Sheardown and J. L. Brash "Protein resistant surfaces formed by chemisorption of thiol terminated poly ethylene oxide on gold: relationship of PEO chain density to protein resistance" Society for Biomaterials 2003.

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H. Chen, H. Sheardown and M.A. Brook "An investigation of the surface properties and biocompatibility of PEO modified silicone rubber" 35<sup>th</sup> Organosilicon symposium 2002.

K. Merrett, C. M. Griffith, M. A. Dube and H. Sheardown "Interactions of corneal cells with TGF  $\beta$ 2 modified poly dimethyl siloxane surfaces" Society for Biomaterials 2002

L.D. Unsworth, H. Sheardown and J. L. Brash "Ellipsometric investigation of the effect of temperature on the chemisorption of thiolated poly (ethylene oxide) on gold: correlation to protein adsorption" Society for Biomaterials 2002

## Books

“Protein Cells and Materials” H. Sheardown and S. Cooper (eds) Brill Academic Publishers (2003).

## Contributions to books

M. Griffith, V. Trinkaus-Randoll, M.A. Watsky, C.Y. Liu, H. Sheardown. “Cornea” in Methods in Tissue Engineering, A. Atalo, R.P. Lanzo (eds) 2002.

M. Griffith, F. Li, C. Lohmann, H. Sheardown, S. Shimmura and D.J. Carlsson. “Tissue engineering of the cornea” in Scaffolding in Tissue Engineering. P. Ma and J. Ellseff (eds) 2003

## Book Chapters

H. Sheardown and M. Saltzman, Novel drug delivery systems for posterior segment ocular disease. To be published in: Angiogenesis in the eye, Barnstable C. (editor) 2004.

## Current Research Projects

### *Artificial Corneas and Corneal Onlays for Restoration of Sight*

*Corneal blindness, a condition that affects millions of patients worldwide, is often treatable by replacing the diseased cornea with a human donor. However, the number of patients of waiting lists has grown dramatically in recent years; many other patients are unsuitable for this treatment or simply do not have donor tissue available. Additionally, the safety of donor tissue is always a consideration. We are currently working on two different models with the ultimate goal of developing an implantable corneal model which can be used either as an artificial cornea or which can be used as a corneal onlay. In one project, synthetic polymers are being used as scaffold materials with the application of appropriate modifications to promote interactions with corneal cells. The second project is focused on a tissue engineered cornea which is based on collagen, the natural polymer that provides the structural component of the normal human cornea.*

### ***Drug Delivery to the Eye***

*While delivery of drugs to the front of the eye is usually quite easily accomplished through the use of drops, delivery of drugs to the back of the eye for the treatment of a variety of debilitating diseases including Age Related Macular Degeneration (AMD) and diabetic retinopathy is complicated by ocular anatomy and physiology. We are looking at various strategies for the targeted delivery of relevant drugs to the appropriate ocular tissues. In one project we are using alginate microspheres for the release of protein drugs. Another project is focused on the use of a MEMs based system for targeted and controlled ophthalmic drug release.*

### ***Modification of Intraocular Lenses for Reduction of Posterior Capsule Opacification***

*Loss of transparency of the lens or cataract is the leading cause of blindness in the world despite the availability of effective surgery. Secondary cataract or posterior capsule opacification (PCO) is the major complication of modern cataract surgery, occurring in between 20 and 40% of patients. This collaborative project is focused on using the ocular signaling molecules involved in PCO formation in conjunction with lens materials to develop novel intraocular lenses which show lower amounts of PCO.*

### ***Surface Modified Polymers to Minimize Fouling***

*Protein fouling is a major cause of complications in numerous biomaterials applications. In the eye, contact lens fouling results in discomfort and end of dryness; in the blood contacting applications, protein fouling and resultant effects lead to thrombus formation which can ultimately occlude the vessel or lead to subsequent deleterious cardiovascular effects. These projects involve the modification of various polymer surfaces with low fouling materials such as poly (ethylene oxide) and phospholipids as well as subsequent functionalization with biologically relevant molecules including heparin and cell adhesion molecules in order to reduce protein adsorption and the resultant effects.*

**SWARTZ, CHRISTOPHER L.E.**  
(Associate Professor)

**Research Interests:** Computer process control, optimization.



**Professional Organizations**

Member:

- Society for Industrial and Applied Mathematics
- American Institute of Chemical Engineers

**Papers in Refereed Journals**

R.D.M. MacRosty, and C.L.E. Swartz, “Dynamic modeling of an Industrial Electric Arc Furnace”, Accepted for publication, Ind. Eng. Chem. Res. (2005).

R. Baker and C.L. E. Swartz, “Rigorous Handling of Input Saturation in the Design of Dynamically Operable Plants”, Ind. Eng. Chem. Res., 43 (18), 5880-5887 (2004).

R. Baker and C.L.E. Swartz “Simultaneous Solution Strategies for Inclusion of Input Saturation in the Optimal Design of Dynamically Operable Plants” Optimization and Engineering, 5, 5-24 (2004).

J.C.C. Young, R. Baker and C.L.E. Swartz “Input Saturation Effects in Optimizing Control – Inclusion Within a Simultaneous Optimization Framework” Comput. Chem. Engng, 28 (8), 1347-1360 (2004).

**Refereed Conference Proceedings**

R.D.M. MacRosty and C.L.E. Swartz, “Optimization as a Tool for Process Improvement in EAF Operations”, Proceedings, AISTech 2005, Charlotte, North Carolina (2005).

R. Baker and C.L.E. Swartz, “Inclusion of Actuator Saturation as Complementarity Constraints in Integrated Design and Control”, 7<sup>th</sup> Int. Symposium of Dynamics and Control of Process Systems (CYCOPS 7), Boston (2004).

M. Soliman, A.K.S. Balthazaar and C.L.E. Swartz, “Modeling and Model-Based control of an Oxygen Delignification Unit”, Control Systems 2004 Conference, Quebec City (2004).

K.G. Dunn and C.L.E. Swartz “On the Use of Controller Parametrization in the Optimal Design of Dynamically Operable Plants” Proceedings of ADCHEM 2003, Hong Kong, (2003).

**Chapters in Books**

C.L.E. Swartz “The Use of Controller Parametrization in the Integration of Design and Control,” in The Integration of Design and Control, P. Seferlis and M. Georgiades (eds) Elsevier, pp 239-263 (2004).

**TAYLOR, PAUL A. (Professor,  
Computing & Software)**

**Research Interests:** computer process control, non linear control, process identification, expert systems and genetic algorithm applications.



**Professional Organizations**

**Papers in Refereed Journals**

A. Esmaili, J.F. MacGregor, P.A. Taylor, "Direct and Two-Step Methods for Closed-Loop Identification: A Comparison of Asymptotic and Finite Data Set Performance", *J. Process Control*, 10, 525-537, (2000).

**THOMPSON, MICHAEL R. (Assistant  
Professor)**

**Research Interests:** polymer processing, extrusion, reactive extrusion, compounding practices and material properties.



**Professional Organizations**

Member:

- Society of Plastics Engineers
- Polymer Processing Society

**Papers in Refereed Journals**

P. A. Moysey and M. R. Thompson, "Investigation of Solids Transport in a Single-Screw Extruder Using a 3-D Discrete Particle Simulation", *Polym. Eng. Sci.*, 44, 2203-2215 (2004)

M. R. Thompson, C. Xi, E. Takacs, M. Tate, J. Vlachopoulos, "Experiments and Flow Analysis of a Micropelletizing Die", *Polym. Eng. Sci.*, 44, 1391-1402 (2004)

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C. Xi, E. Takacs, M. Tate, M.R. Thompson, J. Vlachopoulos, "Study of the Micropelletization Process", *SPE ANTEC* (2003).

M.R. Thompson, J. P. Christiano, "Analysis of Feed Characteristics on the Performance of Groove-Feed Extruders.", *SPE ANTEC*, 47, 190-194 (2001)

K.R. Slusarz, M.R. Thompson, J.P. Christiano, .An Experimental Comparison of the Improved Mixing Obtained from a New Barrier Screw Design., *SPE ANTEC*, 74, 262-266 (2001)

## Patents

M.R. Thompson, J.P. Christiano, .*Extruder Screw.*, Davis-Standard Corporation, US Patent No. 6,176,606, (Jan. 23, 2001)

J.P. Christiano, M.R. Thompson, .*Extruder Screw.*, Davis-Standard Corporation, US Patent No. 6,179,461 (Jan. 30, 2001)

## Current Research Projects

### **MICROMANUFACTURING OF POLYMER COMPOSITES**

*Development of new value-added polymeric materials through extrusion, injection molding and compression molding processes. Our interests lie in exploring the complex interactions that arise between processing history, evolved morphology of the material, and product properties. Current materials under study include clay and graphite nanocomposites, electrical conductive composites, polymer foams, and reinforced polymer foams. Philosophically, our research relies heavily on experiments, however, use of numerical methods is encouraged to complement our analysis*

### **REACTIVE EXTRUSION**

*Over the past decade, this unique field has matured to become a widely employed practice in the industry for polymer modification. The extruder (which is most typically a co-rotating twin screw extruder) acts both as a pump of the molten polymer and as a reactor within which reactions to modify the structure of the polymer occur under controlled conditions. In this project, we are studying the synergies which may be obtained through reactive modification performed concurrently with other processes such as foaming, or polymer blending. As with other projects of my research group, we are looking at the implications of screw design on the process.*

### **POLYMER PROCESSING INVOLVING FOAMED PRODUCTS**

*M.R. Thompson and A.N. Hrymak*

*Polymer foams remain one of the areas in polymer processing that continues to show strong growth. However, the current operating window characteristic of these foaming processes is generally rather small. For sustainable growth, a processor needs to be given tools which will ensure their success and that means stretching the operating window. To reach that goal, improved understanding of the mechanisms involved in polymer foaming is needed. This project studies polymer foaming within injection molding and extrusion equipment through the development of an on-line monitor of polymer rheology during foaming. The mixing of gases into polymer, and its relationship with feedscrew design represent other areas of interest within this work.*

### **DISCRETE MODELLING OF THE SOLIDS-CONVEYING AND MELTING ZONES OF A GROOVE-FEED EXTRUDER**

*Current models of solids-conveying in a conventional single-screw extruder simplify the phenomenon by disregarding the true discrete nature of the medium, instead choosing to treat the solids flow as a continuum that responds isotropically to applied stresses. Occasionally, a lateral stress ratio parameter is incorporated to account for the true anisotropic nature of solid granulates. These models provide a suitable match to trends observed experimentally but lack sufficient resolution to be useful when greater accuracy is required, as in feedscrew design. In addition, these current solids-conveying models prove to be completely unreliable when applied to groove-feed extrusion – a type of extrusion where the output rate is solids-conveying dependent rather than melting dependent as in conventional extrusion. Clearly, a discrete approach is needed to provide the necessary level understanding needed to accurately understand solids-conveying. In addition, melting and solids-conveying are intimately linked in groove-feed extrusion, unlike conventional extrusion where these mechanisms normally follow sequentially. In this project, discrete modelling techniques coupled with experimental observations are used to generate a level of understanding not currently possessed by researchers in our field of plastics extrusion. The goal of the project is to develop an accurate modeling technique capable of assisting rapid, prototype feedscrew development for the extrusion and injection molding industries.*

## **VLACHOPOULOS, JOHN (Professor)**

**Research Interests:** Polymer processing, rheology, finite differences and finite elements, CAD/CAM methods.



### **Professional Organizations**

Member:

- Canadian Society for Chemical Engineering (C.I.C. Fellow)
- American Institute of Chemical Engineers
- Sigma Xi
- Canadian Society of Rheology
- Society of Rheology
- Professional Engineers of Ontario
- Society of Plastics Engineers (Fellow)
- Polymer Processing Society
- Verein Deutscher Ingenieure
- Hellenic Society of Rheology

### **Papers in Refereed Journals**

M. R. Thompson, C. Xi, E. Takacs, M. Tate, J. Vlachopoulos, "Experiments and Flow Analysis of a Micropelletizing Die", *Polym. Eng. Sci.*, 44, 1391-1402 (2004)

M. Thompson, C. Xi, E. Takacs, M. Tate and J. Vlachopoulos "Experiments and Flow Analysis of a Micropelletizing Die" accepted for publication in *Polym. Eng. Sci.* (2003)

D. D'Agostino, E. Takacs and J. Vlachopoulos "Foaming with Polymer Microspheres in Rotational

Molding: The Effect of Coupling Agent" accepted *J. Cell. Plast.* (2003)

V. Sidiropoulos and J. Vlachopoulos "The Aerodynamics of Blown Film Cooling: *Jap. Soc. Polym. Proc. Journal (SciFei Kaku)* 15, 740 (2003)

A. Greco, A. Mafezzoli and J. Vlachopoulos "Simulation of Heat Transfer During Rotational Molding" *Adv. Polym. Tech.* 22, 271 (2003)

J. Vlachopoulos and D. Strutt "Overview: Polymer Processing" *Mats. Sci. Tech.* 19 1153 (2003).

B.I. Chaudhary, E. Takacs and J. Vlachopoulos, "Ethylene Copolymers as Sintering Enhancers and Impact Modifiers for Rotational Molding of Polyethylene", *Polym. Eng. Sci.*, 42, 1359-1369 (2002).

V. Sidiropoulos and J. Vlachopoulos, "Numerical Simulation of Blown Film Cooling, *J. Reinf. Plast. Comp.* 21 (7), 629-637 (2002).

M. Kontopoulou and J. Vlachopoulos, "Melting and Densification of Thermoplastic Powders", *Polym. Eng. Sci.*, 41, 155-169 (2001).

V. Sidiropoulos and J. Vlachopoulos, "Numerical Study of Internal Bubble Cooling (IBC) in Film Blowing", *Int. Polym. Proc.*, 16, 48-53 (2001).

B.J. Chaudhary, E. Takacs and J. Vlachopoulos, "Processing Enhancers for Rotational Molding of Polyethylene", *Polym. Eng. Sci.*, 41, 1731-1742 (2001).

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C. Xi, E. Takacs, M. Tate, M. Thompson and J. Vlachopoulos "Study of the Micropelletization Process" *SPE ANTEC Proceedings*, 278, Nashville, TN (2003)

D. D'Agostina, E. Takacs and J. Vlachopoulos "Effect of coupling Agents on Foaming with Polymer Microspheres in Rotational Molding" *SPE ANTEC Proceedings*, 1205, Nashville, TN (2003)

R.J. Castillo, D. Strutt and J. Vlachopoulos, "Experiments and Simulations with Barrier Screws", *SPE ANTEC Proceedings*, 318-322, San Francisco, CA (2002).

E. Takacs, J. Vlachopoulos and C. Rosenbusch, "Foaming with Microspheres in Rotational Molding", SPE ANTEC Proceedings, 1271-1275, San Francisco, CA (2002).

V. Sidiropoulos, Z. Wahab and J. Vlachopoulos, "Numerical Calculation of Stresses in Film Blowing", SPE ANTEC Proceedings, 86-91, Dallas, TX (2001).

D. Annechini, E. Takacs and J. Vlachopoulos, "Some New Results on Rotational Molding of Metallocene Polyethylene", SPE ANTEC Proceeding, 1291-1295, Dallas, TX (2001).

E. Takacs, J. Vlachopoulos, M. Kontopoulou, E. Voldner and K. Nichols, "Blends of Recycled Polyethylenes and Metallocene Impact Modifiers for Rotational Molding", SPE ANTEC Proceedings, 1296-1301, Dallas, TX (2001).

### Chapters in Books

J. Vlachopoulos and D. Strutt, "Heat Transfer", in SPE Plastics Technicians Toolbox, 2, 21-33, Soc. Plast. Eng., Brookfield, CT (2002).

J. Vlachopoulos and V. Sidiropoulos, "Polymer Film Blowing: Technology and Modelling", Encycl. Mat. Sci. & Tech., 7296-7101, Elsevier (2001).

### Books

J. Vlachopoulos and J. Wagner (Editors), "The SPE Guide on Extrusion Technology and Troubleshooting", Soc. Plast. Eng., Brookfield, CT (2001).

### Current Research Projects

#### **POLYMER PROCESSING**

*Several projects are underway in cooperation with Drs. A.N. Hrymak and M.R. Thompson involving polymer processing. These include studies of polymer pelletization, computer flow simulation, extrusion and injection molding.*

#### **ROTATIONAL MOLDING OF POLYMERS**

##### J. Vlachopoulos

*Rotational molding is a process for the production of hollow plastic parts such as containers, tanks and toys. It involves the tumbling, heating and melting of thermoplastic powder, in a biaxially rotating mold, followed by coalescence, fusion or sintering and cooling. Our research involves experimental work with particle sintering observations under the microscope, rotational molding in uniaxial and biaxial machines accompanied by material characterization and property determination. Some studies are aimed at foams in rotational molding. Attempts are made for development of mathematical models for the description of the various fundamental mechanisms. The ultimate objectives are the expansion of the range of materials used in rotational molding and the improvement of end use properties.*

#### **BLOWN FILM EXTRUSION**

##### J. Vlachopoulos

*Blown film extrusion is the most important process for the production of plastic films. The polymer is melted in an extruder and the hot melt is pumped through a die to form a thin walled tube which is simultaneously axially drawn and radially expanded. We are involved in both computer modelling and experimental work. The ultimate objectives are output increase, defect reduction and the prediction of film properties (dart impact, tear, optics, etc.). It appears that most film properties correlate with the strains and stresses at the freeze line. Defect reduction depends on many factors including die design and bubble control. Output rates depend on cooling capacity and bubble stability. Our methodology combines computer simulations with rheological material characterization.*

## WOOD, PHILIP E. (Professor)

**Research Interests:** Experimental and computational fluid mechanics, heat transfer.



## Professional Organizations

Member:

- Association of Professional Engineers of Ontario
- American Institute of Chemical Engineers
- Canadian Society for Chemical Engineers

## Papers in Refereed Journals

D.R. Woods, P.E. Wood, H. Sheardown and T. Kourti, "Assessing problem solving skills", *Chemical Engineering Education* 35 (4): 290-295 (2001).

S.A. Jaffer, V.L. Bravo, P.E. Wood and A.N. Hrymak, "Experimental validation of numerical simulations of the kneading disk section in a twin screw extruder", *Polymer Eng. & Sci*, 40, pp. 892-901 (2000).

D.A. Johnson and P.E. Wood, "Self-sustained oscillations in opposed impinging jets in an enclosure", *Can. J. Chem. Eng.*, 78, 867-875 (2000).

## ZHU, SHIPING (Professor)

**Research Interests:** Polymer reaction engineering, polymer synthesis, polymerization process modelling, biomaterials, plastic microelectronics.



## Professional Organizations

Member:

- Association of Professional Engineers of Ontario
- Canadian Society for Chemical Engineering
- American Institute of Chemical Engineers
- American Chemical Society

## Papers in Refereed Journals

W. Feng, J. Brash, S. Zhu\* "Non-biofouling materials prepared by atom transfer radical polymerization grafting of 2-methacryloyloxyethyl phosphorylcholine: effect of graft density and chain length on protein repulsion", *Biomaterials*, Jan 2005 (accepted)

H. Eslami, S. Zhu, "Emulsion atom transfer radical polymerization of 2-ethylhexyl methacrylate", *Polymer*, Jan 2005 (accepted)

W. Feng, S. Zhu, J. Brash, K. Ishihara "Adsorption of fibrinogen and lysozyme on silicon wafers grafted with poly(2-methacryloyloxyethyl phosphorylcholine) via surface-initiated atom transfer radical polymerization" *Langmuir*. Jan, 2004 (accepted)

- J. Jin, J.C. Achenback, S. Zhu, Y. Li “Complexation of well-controlled low-molecular weight polyelectrolytes with antisense oligonucleotides” *Colloid Polym. Sci.*, Sept 2004 (accepted)
- F. Alobaidi, S. Zhu, “Synthesis of reactor blends of linear and branched polyethylenes using metallocene/Ni-diimine binary catalyst system in single reactor” *J. Appl. Polym. Sci.*, 96, 2212-2217, 2005.
- A.R. Wang, S. Zhu “Branching and gelation in atom transfer radical polymerization of methyl methacrylate and ethylene glycol dimethacrylate” *Polym Engn Sci.*, **45**, 720-727, 2005
- Y. Wu, P. Liu, B.S. Ong, Srikumar T., N. Zhao, G. Botton, S. Zhu “Controlled orientation of liquid-crystalline polythiophene semiconductors for high-performance organic thin-thin transistors”, *Appl. Phys. Lett.* **86**, 142102-142104, 2005
- S. Faucher, S. Zhu, “Heterogeneous atom transfer radical polymerization of methyl methacrylate at low metal salt concentrations” *Ind. Eng. Chem. Res.*, 44, 677-685, 2005.
- N. Zhao, G.A. Botton, S. Zhu, A. Duft, B. Ong, Y. Wu “Microscopic studies on liquid crystal poly(3,3''-dialkyl-quaterthiophene) semiconductor”, *Macromolecules*, 37, 8307-8312, 2004.
- Y.H. Huang, K. Cao, B.G. Li, S. Zhu “Syndiospecific styrene polymerization with CpTiCl<sub>3</sub>/MAO: effects of the order of reactant addition on polymerization and polymer properties” *J. Appl. Polym. Sci.* 94, 1449-1455, 2004
- W.J. Wang, S. Kharchenko, K. Migler, S. Zhu, “Triple detector array GPC characterization and processing behavior of long chain branched polyethylene prepared by solution polymerization with constrained geometry catalyst”, *Polymer*, **45**, 6495-6505, 2004
- F. Alobaidi, Z. Ye, S. Zhu, “Ethylene polymerization with homogeneous nickel-diimine catalysts – effects of catalyst structure and polymerization conditions on catalyst activity and polymer properties”, *Polymer*, 45, 20, 6823-6829, 2004
- F. Alobaidi, Z. Ye, S. Zhu, “Synthesis of linear low-density polyethylene of ethylene/1-hexene directly from ethylene stock using tandem catalytic system in single reactor” *J. Polym. Sci. Polym. Chem.*, 42, 4327-4336, 2004
- W.J. Wang, Z. Ye, H. Fan, B.G. Li, S. Zhu, “Dynamic mechanical and rheological properties of metallocene-catalyzed long-chain-branched ethylene/propylene copolymers” *Polymer*, 45, 16, 5497-5504, 2004
- Z. Ye, F. Alobaidi, S. Zhu, “Melt rheological properties of branched polyethylenes produced with Pd- and Ni-diimine catalysts” *Macromol. Chem. Phys.*, 205, 7, 897-906, 2004
- Z. Ye, F. Alobaidi S. Zhu, “Synthesis and rheological properties of long chain branched isotactic polypropylene prepared by copolymerization of propylene and non-conjugated dienes:” *Ind. Engr. Chem. Res.*, 43, 2860-2870, 2004
- W. Feng, J. Brash, S. Zhu, “Atom transfer radical grafting polymerization of 2-methacryloyl oxyethyl phosphoryl choline from silicon wafer surfaces” *J. Polym. Sci. Polym. Chem.* **42**, 2931-2942, 2004.
- S. Faucher, S. Zhu, “Location of catalytic site in supported atom transfer radical polymerization”, *Macromol. Rapid Commun.*, 25, 991-994, 2004
- A.R. Wang, S. Zhu, “Heterogeneity features of bulk atom transfer radical polymerization of methyl methacrylate in ampoule reactor” *Macromol. Rapid Comm.*, 25, 9, 925-929, 2004
- Z. Ye, F. Alobaidi, S. Zhu, “A tandem catalyst system for synthesis of polyethylene-1-hexene from ethylene stock”, *Macromol. Rapid Commun.*, 25, 647-652, 2004
- E. Kolodka, S. Zhu, A.E. Hamielec “Rheological and thermomechanical properties of long chain branched polyethylene prepared by slurry polymerization with metallocene catalysts”, *J. Appl. Polym. Sci.*, 92, 307-316, 2004
- J.X.P. Jin, Y. Shen, S. Zhu “Atom transfer radical block copolymerisation of dimethylaminoethyl methacrylate and hydroxyethyl methacrylate” *Macromol. Mat. Eng.* 288, 925 (2003)
- A.R. Wang, S. Zhu “Calculation of monomer conversion and radical concentrations in reversible additional-fragmentation chain transfer radical polymerization” *Macromol. Theory Simul.* 12, 663 (2003)
- Y. Li, S.P. Armes, J.X.P. Jin, S. Zhu “Direct atom transfer radical polymerization of

dimethylaminoethyl methacrylate methchloride quat" *Macromolecules*, 36, 8268 (2003)

H.M. Alsayouri, C. Langheinrich, Y.S. Lin, Z. Ye, S. Zhu "Cyclic chemical vapor deposition modification of straight nanopore alumina membranes" *Langmuir*, 19, 7307-7314, 2003

W. Yu, E.T. Kang, K.G. Neoh, S. Zhu "Controlled grafting of well-defined polymers on hydrogen-terminated silicon substrates by surface-initiated atom transfer radical polymerization", *J. Phys. Chem. B.*, 107, 10198-10205, 2003

Z. Ye, S. Zhu, W.-J Wang, H. Alsayouri Y.S. Lin, G. Weatherly, "Morphological and mechanical properties of nascent polyethylene fibers produced via nano-extrusion polymerization with metallocene catalyst supported on MCM-41 particles", *J Polym. Sci. Polym. Phys.* 41, 2433-2443.

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## Chapters in Books

A.R. Wang, S. Zhu\*, K. Matyjaszewski “ESR Study and radical observation in transition metal mediated polymerization, unified view of atom transfer radical polymerization mechanism”, in “Controlled/Living Radical Polymerization” in *Advances in Controlled/Living Radical Polymerization*, ACS Symposium Series 854, K. Matyjaszewski, ed. ACS Washington DC, Chapt.12, pp.161-179, 2003

## Current Research Projects

### **LIVING/CONTROLLED RADICAL POLYMERIZATION**

We work in the areas of atom-transfer radical polymerization (ATRP) aiming at (1) developing support systems for catalyst recycling, (2) developing continuous processes, and (3) elucidating radical mechanisms. The support systems included physical adsorption and chemical grafting of ATRP catalyst/ligand onto insoluble silica particles and soluble-but-recoverable polymer supports. We also developed a continuous packed-column reactor technology (C-SATRP) for making well-controlled block copolymers. In the fundamental side, we were the first group who observed radical intermediates in ATRP by ESR and thus provided direct support to the debated radical mechanisms. We also investigated the diffusion-controlled reactions in ATRP aimed at improving molecular weight control at high conversion. We collaborate with Professor Krzysztof Matyjaszewski, Carnegie Melon, and Professor Steven Armes, Sussex, in some of the areas.

### **PLASTIC MICROELECTRONICS**

We synthesize and functionalize semi-conductive polymers such as polythiophene for microelectronics applications. Our focuses are on the relationships of polymer chain structure, materials morphology, and carrier mobility and stability of performance of the materials. We particularly emphasize the interfacial problems associated with the materials. We collaborate with Professor Gianluigi Botton and Gu Xu in Materials and Jamal Deen in Electrical and Computer Engineering in this area.

### **MODELING POLYMERIZATION PROCESSES**

We develop mathematical models for various polymerization processes. Recently, we focused on branched polymers as well as those produced by living/controlled radical polymerization processes. We collaborate with Professor Hidataka Tobita Fukui and Eduardo Vilvado-Lima UNAM in some of the areas.

### **OLEFIN POLYMERIZATION WITH SINGLE SITE TYPE CATALYSTS**

We work in the areas of (1) preparation and characterization of long chain branched (LCB) polyethylene, and (2) control of polyethylene morphology by nano-tube particles. We made LCBed PEs in high temperature solution polymerization using a CSTR technology. The samples showed significant shear thinning properties. We investigated ethylene copolymerization with propylene and octene. By comparing the comonomer reactivities to that of in-situ generated PE macromonomer, we proposed a same-site branching mechanism, that is, PE macromonomer is incorporated into PE backbone chain at the same site as it is generated. We developed various methods for making more LCBs, that include binary catalyst systems and two-step processes. Recently, we work on using nano-tube particles as support for metallocene catalysts to prepare extended chain crystal PE fibers. A perfect ECC PE fiber is expected to have a mechanical strength competitive to steel.

### **POLYMER GRAFTING FOR NON BIO-FOULING SURFACES AND POLYELECTROLYTES FOR NON-VIRAL GENE DELIVERIES**

We graft bio-compatible polymers such as 2-methacryloyloxy ethyl phosphorylcholine (MPC) onto inorganic/organic surfaces by ATRP methods. These polymer-modified surfaces have good protein repulsion properties to avoid bio-fouling. We collaborate with Professor John Brash in this area. We also work on preparing well-defined polyelectrolytes using ATRP for non-viral gene/drug delivery purposes. For example, polymer products of 2-(dimethylamino)ethyl methacrylate can complex with DNA or oligonucleotides that facilitates transfection. We collaborate with Professor Yingfu Li in Biochemistry McMaster in this area.