

PROFESSIONAL ACTIVITIES (1995-present)

INTERNATIONAL:

Scientific Committee, Chemometrics in Analytical Chemistry Conference, 2008 and 2010
 Editor, *Chemometrics and Intelligent Laboratory Systems*, 1998-2006.
 EAS Chemometrics Award Selection Committee (2005/6/7), 2004-6.
 Kowalski Award Selection Committee (2004), *Journal of Chemometrics*, 2004.
 Assistant Editor, *Chemometrics and Intelligent Laboratory Systems*, 1996-7.
 Editorial Advisory Board, *Analytica Chimica Acta*, 1997-2000.
 Consultant, Union Carbide, South Charleston, West Virginia, May 20, 1998.
 Review Panel Member, U.S. National Science Foundation EPSCoR (Experimental Program to Stimulate Competitive Research) in Idaho, Sept. 14-16, 1997, Moscow, Idaho.

NATIONAL:

Scientific Committee, 2009 Atlantic Omics Symposium, 2009.
 External Ph.D. Thesis Examiner for Xiumei Han, Department of Chemistry, Queen's University, March 30, 2007.
 Analytical Division Program Chair, CSC Conference, 2006.
 Consultant, Osler, Hoskin & Harcourt LLP, Ottawa, August, 2003.
 External Ph.D. Thesis Examiner for Suzanne Schreyer, Department of Chemistry, University of Waterloo, August 11, 2000.
 External Ph.D. Thesis Appraiser for Lan Nang Bui, Department of Chemistry, University of Toronto, January, 1999.
 Executive Member-at-Large, Analytical Chemistry Division of the Chemical Institute of Canada (CIC), 1992-95.

SERVICE TO THE UNIVERSITY/DEPARTMENT:

Departmental Committees:

Chemistry Chair Advising Committee (2010-)
 Curriculum Renewal Committee (Chair, 2008-)
 Academic Advisor (2007-)
 Safety Committee (2007-)
 Graduate Studies Committee (2004-2006)
 (1997-2002)
 (1991 - 1995)
 Faculty Search Committee:
 Member, UFA Search (2006)
 Chair, Phys. Chem. Instructor (2006)
 Chair, First-Year Instructor (2005)
 Member, UFA Search (2005)
 Chair, Limited Term Search (2005)
 Member, Comp. Chem. Search (2005)
 Instructor Workload Committee (2004)
 Appointments and Nominations (Co-chair, 2000-2002)
 (member, 2002)
 Library Representative (07/2001 – 12/2001)
 Committee on Computing and Related Support (1998)
 Outreach and Related Activities (1998)
 Strategic Planning Committee (1996-1998)
 Seminar Coordinator (1993 - 1995)

University/Faculty Committees:

Curriculum Committee (2008-)
 Tenure and Promotion Committee (2007- 10, Chair 09/10)
 Ad hoc Committee on On-line Evaluations (Chair, 2008)
 Mathematics/Statistics Chair Advisory Committee (2005)
 Faculty of Graduate Studies Advisory Committee on
 M.Sc. in Computational Biology/Bioinformatics (2005)
 Travel Expenses Advisory Committee (2000-2002)
 Psychology Chair Advisory Committee (Chair, 2002)
 Killam Post-Doctoral Fellowship Committee (2000-2001)
 Senate Library Committee (07/2001-12/2001)
 Biology Chair Advisory Committee (2000)
 Summer Fellowship Committee (1997-1999)
 Oceanography Chair Advisory Committee (1995)

Other:

Director of Trace Analysis Research Centre (TARC) (2008-)
 Dalhousie University Recording Teaching Accomplishment Workshop Series, Panel Member, May 20, 2010
 Science Fair Judge, Millwood High School, May 18, 2010.
 Dalhousie University Promotion and Tenure Workshop, Panel Member, May 12, 2010
 Student Evaluation Streamlining (2007)
 Liaison, Department of Education Advanced Studies Program (2001)
 Chemistry Coordinator, Dalhousie High School Week, August 25-29, 2000
 Panel Member, Henson College "Returning to Learning" Orientation Program, Sept. 3, 1997.
 Participant in the High School Week Program, 1992-1995.

TEACHING SUMMARY

DALHOUSIE COURSES:

Year	Course Title and Number	No. of Students
2009/2010	Engineering Chemistry 1, Chem 1021A	278
2008/2009	Introductory Chemistry Related to Human Health, Chem 1410A	37
	Introductory Chemistry Related to Human Health, Chem 1410A (Distance – Michener Institute)	45
	Chemometrics, Chem 4205A/6205A	27
2007/2008	Introductory Chemistry Related to Human Health, Chem 1410A	40
	Introductory Chemistry Related to Human Health, Chem 1410A (Distance – Michener Institute)	50
	Chemometrics, Chem 4205B/6205B	26
2006/2007	Introductory Chemistry Related to Human Health, Chem 1410A	35
	Introductory Chemistry Related to Human Health, Chem 1410A (Distance – Michener Institute)	46
	B-term - Sabbatical	
2005/2006	Introductory Chemistry Related to Human Health, Chem 1410A	39
	Instrumental Methods of Analysis, Chem 3202B	24
2004/2005	Introductory Chemistry Related to Human Health, Chem 1410A	30
	Chemometrics, Chem 4205A/6205A	29
	Instrumental Methods of Analysis, Chem 3202B	25
2003/2004	A-term – Sabbatical	
	General Chemistry, Chem 1012B	115
	Instrumental Methods of Analysis, Chem 3202B	18
2002/2003	Introductory Chemistry Related to Human Health, Chem 1410A	67
	Chemometrics, Chem 4205A/6205A	16
	B-term - Sabbatical	
2001/2002	Introductory Chemistry Related to Human Health, Chem 1410A	78
	Introductory Analytical Chemistry, Chem 2201A	60
	Introductory Analytical Chemistry, Chem 2201B	18
2000/2001	Introductory Analytical Chemistry, Chem 2201A	57
	Chemometrics, Chem 4205A/6205A	8
	Instrumental Methods of Analysis, Chem 3202B	25
1999/2000	General Chemistry, Chem 1011A	98
	Introductory Analytical Chemistry, Chem 2201A	46
	General Chemistry, Chem 1012B	90
1998/99	Introductory Analytical Chemistry, Chem 2201A	44
	General Chemistry, Chem 1012B	83
	Chemometrics, Chem 6205B	4
1997/98	General Chemistry, Chem 1011A	55
	General Chemistry, Chem 1012B	55
	Introductory Analytical Chemistry, Chem 2201B	30
1996/97	A-term - Sabbatical	
	Introductory Analytical Chemistry, Chem 2201B	56
	Chemometrics, Chem 6205B	4
1995/96	Introductory Analytical Chemistry, Chem 2201A	48
	Chemometrics, Chem 6205A	6
	B-term - Sabbatical	
1994/95	General Chemistry, Chem 1010R (A-term)	68
	Instrumental Methods of Analysis, Chem 3202B	34
1993/94	Advanced General Chemistry, Chem 1500R (A-term)	33
	Instrumental Methods of Analysis, Chem 3202B	29
	Chemometrics, Chem 6205B	10
1992/93	Introductory Analytical Chemistry, Chem 2201A	25
	Instrumental Methods of Analysis, Chem 3202B	19
	Chemometrics, Chem 6205A	7
1991/92	General Chemistry, Chem 1010R	93
	Introductory Analytical Chemistry, Chem 2201B	70
1990/91	General Chemistry, Chem 1010R	78
1989/90	General Chemistry, Chem 1100R	113
	Electronic Instrumentation for Scientists, Chem 6280A (1/3)	10

STUDENTS AND RESEARCH ASSOCIATES SUPERVISED

<u>Name</u>	<u>Years</u>	<u>Program</u>	<u>Last Known Status</u>
Graduate Students:			
Joseph Boutilier	09-	M.Sc.	Continuing
Siyuan Hou	07-	Ph.D.	Continuing
Robert M. Flight	04-09	Ph.D.	Research Associate, Dalhousie University
Hannes Hochreiner	04-08	Ph.D.	Scientist, Merck, Darmstadt, Germany
Tobias K. Karakach	00-02	M.Sc.	
	02-06	Ph.D.	Research Scientist, NRC-IMB, Halifax
Marc N. Leger	99-01	M.Sc.	
	01-04	Ph.D.	Assistant Professor, St. F.X. University, NS
Lorenzo J. Vega-Montoto	98-01	M.Sc.	
	01-05	Ph.D.	Post-doctoral Fellow, Texas A&M University
Praneeth Edirisinghe	99-01	M.Sc.	Withdrew
Christopher D. Brown	96-00	Ph.D.	Research Scientist, Ahura Corporation, Boston, MA
Kelli M. Miller	98-99	M.Sc.	Withdrew
Mitchell T. Lohnes	96-98	M.Sc.	XwaveSolutions. Halifax, NS
Stephanie A. Mehlman	95-98	M.Sc.	Physical Scientist, Environment Canada, Dartmouth, NS
Darren T. Andrews	92-97	Ph.D.	Instructor, Nova Scotia Community College, Sydney, NS
Stephen G. Hughes	91-95	Ph.D.	Diagnostic Chemicals Ltd. Charlottetown, PEI
Stephen J. Vanslyke	90-94	Ph.D.	Research Scientist, InLight Solutions, Albuquerque, NM
Nils G. Sundin	89-91	M.Sc.	Completed Ph.D. at University of Massachusetts
Undergraduate Students:			
Anthony Tarasuk	09/10	B.Sc. (Honours)	Continuing
Alexander Safatli	2009	B.Sc. (USRA)	Continuing
Bjorn Wielens	2009	B.Sc. (USRA)	Continuing
	2008	B.Sc. (USRA)	
Joseph Boutilier	08-09	B.Sc. (Honours)	Entering M.Sc. program at Dalhousie
	2007	B.Sc. (Summer)	
Jennifer Onochie	2008	B.Sc. (Summer)	Continuing
Yazeed Sobaih	2006	B.Sc. (USRA)	Transferred to Commerce
Kaitlyn MacIntosh	2005	B.Sc. (Summer)	Completed degree; entered Pharmacy at University of Alberta
Chantelle Taylor	02,03,04	B.Sc. (Summer)	Completed degree; entered B.Ed. program
Nicholas Spinney	2001	B.Sc.	Completed degree
Mike Bidinosti	2000	B.Sc. (USRA)	Completed B.Sc. (Brandon/Manitoba))
Robyn Ngan	2000	B.Sc. (Summer)	Completed B.Sc.
Sreeja Nair	98-99	B.Sc.(Honours)	Computer Science at Dalhousie
John MacKinnon	97-98	B.Sc.(Honours)	Computer training at St. F.X
Jennifer Walsh	96-97	B.Sc. (Project)	Pursued Chemical Engineering at University of Waterloo
Marcel Moulaison	94-95	B.Sc. (Honours)	Quality Control Scientist, SepraChem, Windsor, NS
Huiming Zheng	94-95	B.Sc. (Honours)	Completed Law degree at York University
Tracy Morgan	94-95	B.Sc. (Project)	Lab Manager, VWR , Weston, ON
Siew Bang Cheng	93-94	B.Sc. (Honours)	Pursued graduate studies at the University of Alberta
Michael J. Little	93-94	B.Sc. (Project)	M.Sc. (Concordia), Scientist for Boehringer-Ingelheim, Montreal
Tara Paton	92-93	B.Sc. (Honours)	Pursued graduate studies in Pharmacology at Dalhousie University
Mark Beasy	91-92	B.Sc. (Honours)	Pursued graduate studies at the University of Guelph
Todd Wood	91-92	B.Sc. (Honours)	M.Sc. (Waterloo), Instrument Operator, University of Victoria
Craig MacDonald	90-91	B.Sc. (Honours)	Pursued studies at the Technical University of Nova Scotia
Kelly Boutilier	90-91	B.Sc. (Project)	Lab Instructor, Acadia University
Mike Bowdridge	1990	Summer Student	B.Sc. (Hons.) (Dalhousie), pursued graduate studies at UBC
Crystal Hogeboom	1990	(USRA)	Pursued studies in Pharmacy
Kevin Bateman	89-90	B.Sc. (Honours)	M.Sc. (Waterloo), Ph.D. (Dalhousie), Merck-Frosst, Montreal

<u>Name</u>	<u>Years</u>	<u>Program</u>	<u>Last Known Status</u>
Post-doctoral Researchers and Visiting Scientists:			
Dr. Michal Daszykowski	2009	Visiting Scientist	Continuing appointment, University of Silesia, Katowice, Poland
Dr. Ivana Stanimirova	2009	Visiting Scientist	Continuing appointment, University of Silesia, Katowice, Poland
Dr. Suzanne Schreyer	00-01	PDF	Research Scientist, Polychromix
Dr. Knut Baumann	1998	Visiting Scientist	Continuing appointment (Habilitation) at the University of Wuerzburg
Dr. Ji-Hong Wang	97-98	PDF	Postdoctoral Fellow at Clarkson University
Dr. Carlos Lucasius	93-95	PDF (NSERC)	Private consultant, Toronto

RESEARCH GRANTS AND CONTRACTS

<u>Agency</u>	<u>Type</u>	<u>Amount (\$ Cdn)</u>	<u>Period</u>	<u>Title</u>
NSERC ¹	Discovery	\$43,000/yr	'08-13	"New Chemometric Tools for Chemistry and Systems Biology"
MITACS ²	Internship	\$15,000	'07-08	"DNA Microarray Studies of the Effect of Diet on Halibut"
NSERC ¹	Discovery	\$42,300/yr	'03-08	"Fundamental and Applied Studies in Chemometrics"
Precarn ³	Contract	\$27,500/yr	'04-05	"Intelligent Advanced Environmental Monitoring Systems"
TSRI ⁴	Research Contract	\$91,000/yr	'99-02	"An Investigation of the PACs Present in the Atmospheric Environment"
Dow ⁵	Research	\$36,900	'01-02	"Optimal Preprocessing in Multivariate Calibration"
NSERC ¹	Research	\$39,900/yr	'99-03	"Fundamental and Applied Studies in Chemometrics"
Dow ⁵	Research	\$31,040	'99-00	"Optimal Preprocessing in Multivariate Calibration"
NSERC ^{1,6}	Group Strategic	\$75,625/yr	'95-99	"The Separation and Identification of Polycyclic Aromatic Compounds in Petroleum Related Samples"
NSERC ¹	Research	\$28,200/yr	'95-99	"Fundamental and Applied Studies in Chemometrics"
Dow ⁴	Research	\$14,400	1998	"Optimal Preprocessing in Multivariate Calibration"
DUIC ⁶	Research	\$5,000	'96-97	"Chemometrics"
NSERC ^{1,5}	Equipment	\$75,765	'95-96	"The Separation and Identification of Polycyclic Aromatic Compounds in Petroleum Related Samples"
NSERC ¹	Research	\$24,000/yr	'92-95	"Chemometrics and Chemical Sensors"
NSERC ¹ / Killam ⁸	Postdoctoral Fellowship	\$29,000/yr	'93-95	"Genetic Algorithms and Chemometrics" with Dr. Carlos B. Lucasius
RDFS ⁹	Research	\$2,500	'93-94	"Data Acquisition System for a Diode Array Chromatography Detector" (with R.L. White)
NSERC ^{1,10}	Equipment	\$72,480	'93-94	"Workstation Cluster for Research in Chemistry"
NRC ¹¹	Contract	\$7,000	'91-93	"Chemometrics and Multivariate Statistical Methods"
NSERC ¹	Operating	\$23,000/yr	'90-92	"Studies in Chemometrics and Chemical Sensors"
NSERC ¹	Equipment	\$19,764	'90-91	"Chemical Acoustic Emission Signal Collection Apparatus"
RDFS ⁹	Research	\$5,000	'90-91	"Automated Optimization and Response Modeling in Chemistry"
RDFS ⁹	Research	\$15,000	'89-90	"Fundamental and Applied Studies in Chemometrics"

Notes:

1. Natural Sciences and Engineering Research Council of Canada grant.
2. Mathematics of Information Technology and Complex Systems (Canadian NCE).
3. Precarn, Inc. contract through Avensys, Inc.: a multi-university project.
4. Health Canada Toxic Substances Research Initiative. Co-held with L. Ramaley (PI) and R.D. Guy.
5. Dow Chemical Company, Midland, Michigan.
6. Co-held with R.J. Boyd (PI), R.D. Guy and L. Ramaley.
7. Dalhousie University Innovations in Chemistry grant.
8. NSERC/Dalhousie Killam Foundation Post-doctoral Fellowship co-awarded for Dr. C.B. Lucasius.
9. Research and Development in the Sciences grant, Dalhousie University.
10. Co-held with six other applicants from the Chemistry Department.
11. National Research Council, Halifax branch (Institute for Marine Biosciences).

RESEARCH PUBLICATIONS AND PRESENTATIONS

A. Refereed Journal Publications:

- A68. T.K. Karakach, R.M. Flight, S.E. Douglas and P.D. Wentzell, "An Introduction to DNA Microarrays for Gene Expression Analysis", *Chemom. Intell. Lab. Syst.*, (2010), doi:10.1016/j.chemolab.2010.04.003. In press.
- A67. R.M. Flight and P.D. Wentzell, "Preliminary Exploration of Time-Course DNA Microarray Data with Correlation Maps", *OMICS*, **14**, 99-107 (2010). (doi: 10.1089/omi.2009.0096)
- A66. R. Tauler, M. Viana, X. Querol, A. Alastuey, R.M. Flight, P.D. Wentzell, P.K. Hopke, "Comparison of the Results Obtained by Four Receptor Modeling Methods in Aerosol Source Apportionment Studies", *Atmosph. Environ.*, **43**, 3989-3997 (2009). (doi: 10.1016/j.atmosenv.2009.05.018)
- A65. R.M. Flight and P.D. Wentzell, "Potential Bias in GO::TERMFINDER", *Brief. Bioinform.*, **34**, 289-294 (2009). (doi: 10.1093/bib/bbn054)
- A64. T.K. Karakach, P.D. Wentzell and J.A. Walter, "Characterization of the Measurement Error Structure in 1D ¹H NMR Data for Metabolomics Studies", *Anal. Chim. Acta*, **636**, 163-174 (2009). (doi:10.1016/j.aca.2009.01.048)
- A63. H. Hochreiner, M. Cada and P.D. Wentzell, "Modeling of the Response of a Long-Period Fiber Grating to Ambient Refractive Index Change in Chemical Sensing Applications", *IEEE J. Lightwave Technol.*, **26**, 1986-1992 (2008).
- A62. T.K. Karakach, R.M. Flight and P.D. Wentzell, "Bootstrap Method for the Estimation of Measurement Uncertainty in Spotted Dual-Color DNA Microarrays", *Anal. Bioanal. Chem.*, **389**, 2125-2141 (2007).
- A61. T.K. Karakach and P.D. Wentzell, "Methods for Estimating and Mitigating Errors in Spotted, Dual-color DNA Microarrays", *OMICS*, **11**, 186-199 (2007).
- A60. P.D. Wentzell, T.K. Karakach, S. Roy, M.J. Martinez, C.P. Allen and M. Werner-Washburne, "Multivariate Curve Resolution of Time Course Microarray Data", *BMC Bioinformatics*, **7**, 343 (2006). (19 pages)
- A59. L. Vega-Montoto and P.D. Wentzell, "Approaching the Direct Exponential Curve Resolution Algorithm from a Maximum Likelihood Perspective", *Anal. Chim. Acta*, **556**, 383-399 (2006).
- A58. A.D. Aragon, G.A. Quinones, C. Allen, J. Thomas, S. Roy, G.S. Davidson, P.D. Wentzell, B. Millier, J.E. Jaetao, A.L. Rodriguez and M. Werner-Washburne, "An Automated, Pressure-Driven Sampling Device for Harvesting from Liquid Cultures for Genomic and Biochemical Analysis", *J. Microbiol. Meth.*, **65**, 357-360 (2006).
- A57. L. Vega-Montoto and P.D. Wentzell, "Mathematical Improvements to Maximum Likelihood Parallel Factor Analysis: Experimental Studies", *J. Chemom.*, **19**, 236-252 (2005).
- A56. L. Vega-Montoto, H. Gu and P.D. Wentzell, "Mathematical Improvements to Maximum Likelihood Parallel Factor Analysis: Theory and Simulations", *J. Chemom.*, **19**, 216-235 (2005).
- A55. P.D. Wentzell and T.K. Karakach, "DNA Microarrays: Is there a role for Analytical Chemistry?", *Analyst*, **130**, 1331-1336 (2005). (Cover article)
- A54. M. Schuermans, I. Markovskiy, P.D. Wentzell and S. Van Huffel, "On the Equivalence between Total Least Squares and Maximum Likelihood PCA", *Anal. Chim. Acta*, **544**, 254-267 (2005).
- A53. M.N. Leger, L. Vega-Montoto and P.D. Wentzell, "Methods for Systematic Investigation of Measurement Error Covariance Matrices", *Chemom. Intell. Lab. Syst.*, **77**, 181-205 (2005).
- A52. M.J. Martinez, S. Roy, A.B. Archuleta, P.D. Wentzell, S.S. Anna-Arriola, A.L. Rodriguez, A.D. Aragon, G. Quinones, C. Allen, and M. Werner-Washburne, "Genomic Analysis of Stationary Phase and Exit in *Saccharomyces Cerevisiae*: Gene Expression and Identification of Novel Essential Genes", *Mol. Biol. Cell*, **15**, 5295-5305 (2004).
- A51. M.N. Leger and P.D. Wentzell, "Maximum Likelihood Principal Components Regression on Wavelet-Compressed Data", *Appl. Spectrosc.*, **58**, 855-862 (2004).
- A50. L. Vega Montoto and P.D. Wentzell, "Maximum Likelihood Parallel Factor Analysis (MLPARAFAC)", *J. Chemomet.*, **17**, 237-253 (2003).
- A49. P.D. Wentzell and L. Vega Montoto, "Comparison of Principal Components Regression and Partial Least Squares Regression through Complex Mixture Simulation", *Chem. Intell. Lab. Syst.*, **65**, 257-279 (2003).
- A48. S.K. Schreyer, M. Bidinosti and P.D. Wentzell, "Application of Maximum Likelihood Principal Components Regression to Fluorescence Emission Spectra", *Appl. Spectrosc.*, **56**, 789-796 (2002).
- A47. M.N. Leger and P.D. Wentzell, "Dynamic Monte Carlo Self-Modeling Curve Resolution Method for Multicomponent Mixtures", *Chemom. Intell. Lab. Syst.*, **62**, 171-188 (2002).
- A46. P.D. Wentzell, S.S. Nair and R.D. Guy, "Three-Way Analysis of Fluorescence Spectra of Polycyclic Aromatic Hydrocarbons with Quenching by Nitromethane", *Anal. Chem.*, **73**, 1408-1415 (2001).
- A45. C.D. Brown, L. Vega-Montoto and P.D. Wentzell, "Derivative Preprocessing and Optimal Corrections for Baseline Drift in Multivariate Calibration", *Appl. Spectrosc.*, **54**, 1055-1068 (2000).
- A44. C.D. Brown and P.D. Wentzell, "A Modification to Window Target-Testing Factor Analysis Using a Gaussian Window", *Chemom. Intell. Lab. Syst.*, **51**, 3-7 (2000).
- A43. P.D. Wentzell, D.T. Andrews, J.M. Walsh, J.M. Cooley and P. Spencer, "Estimation of Hydrocarbon Types in Light Gas Oils and Diesel Fuels by Ultraviolet Absorption Spectroscopy and Multivariate Calibration", *Can. J. Chem.*, **77**, 391-400 (1999).

- A42. M.T. Lohnes, R.D. Guy and P.D. Wentzell, "Window Target-Testing Factor Analysis: Theory and Application to the Chromatographic Analysis of Complex Mixtures with Multiwavelength Fluorescence Detection", *Anal. Chim. Acta*, **389**, 95-113 (1999).
- A41. C.D. Brown and P.D. Wentzell, "Hazards of Digital Smoothing Filters as a Preprocessing Tool in Multivariate Calibration", *J. Chemomet.*, **13**, 133-152 (1999).
- A40. P.D. Wentzell and M.T. Lohnes, "Maximum Likelihood Principal Component Analysis with Correlated Measurement Errors: Theoretical and Practical Considerations", *Chemom. Intell. Lab. Syst.*, **45**, 65-85 (1999).
- A39. P.D. Wentzell, J.-H. Wang, L.F. Loucks and K.M. Miller, "Direct Optimization of Self-Modeling Curve Resolution: Application to the Kinetics of the Permanganate-Oxalic Acid Reaction", *Can. J. Chem.*, **76**, 1144-1155 (1998).
- A38. S.A. Mehlman, P.D. Wentzell and V.L. McGuffin, "Prediction of Simple Physical Properties of Mixed Solvent Systems by Artificial Neural Networks", *Anal. Chim. Acta*, **371**, 117-130 (1998).
- A37. R.D. Guy, L. Ramaley and P.D. Wentzell, "An Experiment in the Sampling of Solids for Chemical Analysis", *J. Chem. Educ.*, **75**, 1028-1033 (1998).
- A36. D.T. Andrews and P.D. Wentzell, "Applications of Maximum Likelihood Principal Component Analysis: Incomplete Data Sets and Calibration Transfer", *Anal. Chim. Acta*, **350**, 341-352 (1997).
- A35. P.D. Wentzell, D.T. Andrews and B.R. Kowalski, "Maximum Likelihood Multivariate Calibration", *Anal. Chem.*, **69**, 2299-2311 (1997).
- A34. P.D. Wentzell, D.T. Andrews, D.C. Hamilton, K. Faber and B.R. Kowalski, "Maximum Likelihood Principal Component Analysis", *J. Chemomet.*, **11**, 339-366 (1997).
- A33. D.T. Andrews, L. Chen, P.D. Wentzell and D.C. Hamilton, "Comments on the Relationship Between Principal Components Analysis and Weighted Regression for Bivariate Data Sets", *Chemom. Intell. Lab. Syst.*, **34**, 231-244 (1996).
- A32. K.B. Thurbide, P.D. Wentzell and W.A. Aue, "Acoustic Flame Detector for Gas Chromatography", *Anal. Chem.*, **68**, 2758-2765 (1996).
- A31. M.J. Little and P.D. Wentzell, "Evaluation of Acoustic Emission as a Means of Carbonate Detection", *Anal. Chim. Acta*, **309**, 283-292 (1995).
- A30. S.G. Hughes and P.D. Wentzell, "Evolving Projection Analysis of Multicomponent Mixtures", *Talanta*, **42**, 1361-1371 (1995).
- A29. P.D. Wentzell, S.G. Hughes and S.J. Vanslyke, "Parallel Kalman Filters for Peak Purity Analysis: Extensions to Non-Ideal Detector Response", *Anal. Chim. Acta*, **307**, 459-470 (1995).
- A28. P.D. Wentzell, N.G. Sundin and C. Hogeboom, "Response Surfaces for the Determination of Arsenic(III) by Hydride Generation Atomic Absorption Spectrometry and Flow Injection", *Analyst*, **119**, 1403-1411 (1994).
- A27. S.G. Hughes, E.L. Taylor, P.D. Wentzell, R.F. McCurdy and R.K. Boss, "Models for Conductance Measurements in the Quality Assurance of Water Analysis", *Anal. Chem.*, **66**, 830-835 (1994).
- A26. S.J. Vanslyke and P.D. Wentzell, "Limitations of Evolving Principal Components Innovation Analysis for Peak Purity Detection in Chromatography", *Chemom. Intell. Lab. Syst.*, **20**, 183-195 (1993).
- A25. P.D. Wentzell, M.R. Bowdridge, E.L. Taylor and C. MacDonald, "Random Walk Simulation of Flow Injection Analysis: Evaluation of Dispersion Profiles", *Anal. Chim. Acta*, **278**, 293-306 (1993).
- A24. R.L. White, P.D. Wentzell, M.A. Beasy, D.S. Clark and D.W. Grund, "Taxonomy of *Amanita* Mushrooms by Pattern Recognition of Amino Acid Chromatographic Data", *Anal. Chim. Acta*, **277**, 333-346 (1993).
- A23. M. Lopez-Nieves, P.D. Wentzell and S.R. Crouch, "Continuous Flow Method for the Determination of Aromatic Aldehydes", *Anal. Chim. Acta*, **258**, 253-258 (1992).
- A22. I.H. Brock, O. Lee, K.A. Soulsbury, P.D. Wentzell, D.B. Sibbald and A.P. Wade, "Toolbox for Chemical Acoustic Emission Data Acquisition and Analysis", *Chemom. Intell. Lab. Syst.*, **12**, 271-290 (1992).
- A21. P.D. Wentzell and S.J. Vanslyke, "Parallel Kalman Filter Networks for Kinetic Methods of Analysis", *Anal. Chim. Acta*, **257**, 173-181 (1992).
- A20. S.J. Vanslyke and P.D. Wentzell, "Real-Time Principal Components Analysis Using Parallel Kalman Filter Networks for Peak Purity Analysis", *Anal. Chem.*, **63**, 2512-2519 (1991).
- A19. T.G. Crowther, A.P. Wade, P.D. Wentzell and R. Gopal, "Characterization of Acoustic Emission from an Electrolysis Cell", *Anal. Chim. Acta*, **254**, 223-234 (1991).
- A18. P.D. Wentzell, O. Lee and A.P. Wade, "Comparison of Pattern Recognition Descriptors for Chemical Acoustic Emission Analysis", *J. Chemomet.*, **5**, 389-403 (1991).
- A17. P.D. Wentzell and N.G. Sundin, "Versatile Pump Controller for Continuous Flow Methods", *Anal. Instrum.*, **19**, 167-179 (1991).
- A16. A.P. Wade, D.B. Sibbald, M.N. Bailey, R.M. Belchamber, S. Bittman, J.A. MacLean and P.D. Wentzell, "An Analytical Perspective on Acoustic Emission", *Anal. Chem.*, **63**, 497A-507A (1991).
- A15. P.D. Wentzell, S.J. Vanslyke and K.P. Bateman, "Evaluation of Acoustic Emission as a Means of Quantitative Chemical Analysis", *Anal. Chim. Acta*, **246**, 43-53 (1991).
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- A8. P.D. Wentzell, M.J. Hatton, P.M. Shiundu, R.M. Ree, A.P. Wade, D. Betteridge and T.J. Sly, "Computer-Controlled Apparatus for Automated Development of Continuous Flow Methods", *J. Automat. Chem.*, **11**, 227-234 (1989).
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- A6. P.D. Wentzell, M.I. Karayannis and S.R. Crouch, "Simultaneous Kinetic Determinations with the Kalman Filter", *Anal. Chim. Acta*, **224** 263-274 (1989).
- A5. D.B. Sibbald, P.D. Wentzell and A.P. Wade, "Display Methods for Dendrograms", *Trends in Anal. Chem.*, **8**, 289-291 (1989).
- A4. P.D. Wentzell, A.P. Wade and S.R. Crouch, "Modeling Chemical Response Surfaces with the Kalman Filter", *Anal. Chem.*, **60**, 905-911 (1988).
- A3. P.D. Wentzell, T.P. Doherty and S.R. Crouch, "Frequency Response of Initial Point Least Squares Polynomial Filters", *Anal. Chem.*, **59**, 367-371 (1987).
- A2. P.D. Wentzell and S.R. Crouch, "Comparison of Reaction-Rate Methods of Analysis for Systems Following First-Order Kinetics", *Anal. Chem.*, **58**, 2855-2858 (1986).
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B. Manuscripts Submitted for Publication:

- B1. R.M. Flight, J. Boutillier and P.D. Wentzell, "Reproducibility of Gridding and Flagging in Microarray Image Processing", *Bioinformatics*, submitted for publication, Feb. 19, 2010.

C. Other Refereed Contributions:

- C3. P.D. Wentzell, "Other Topics in Soft-Modeling: Maximum Likelihood Based Soft-Modeling Methods", in *Comprehensive Chemometrics*, S.D. Brown, R. Tauler and B. Walczak, Eds.; Elsevier, Amsterdam, 2009; vol **2**, pp. 507-558.
- C2. P.D. Wentzell and C.D. Brown, "Signal Processing in Analytical Chemistry", in the *Encyclopedia of Analytical Chemistry*, R.A. Meyers, Ed.; Wiley, Chichester, UK; 2000; vol **11**, pp. 9764-9800.
- C1. P.D. Wentzell, S.J. Vanslyke and S.G. Hughes, "Parallel Digital Filters for Ordered Spectral Data Sets", in *Computer-Enhanced Analytical Spectroscopy*, (S.D. Brown, Ed.); Wiley: New York; 1996; pp. 139-173.

D. Non-Refereed Contributions:

- D4. P.D. Wentzell, Book Review of "Microarrays: Preparation, Microfluidics, Detection Methods, and Biological Applications", K. Dill, R.H. Liu and P. Grodzinski, Eds.; Springer, New York, 2009; *J. Am. Chem. Soc.*, **131**, 13181-13182 (2009).
- D3. H. Hochreiner, M. Cada and P.D. Wentzell, "Tuning the Response of Long-Period Fiber Gratings for Chemical Sensing Applications", in *Next-Generation Spectroscopic Technologies*, C.D. Brown, M.A. Druy and J.P. Coates, Eds., *Proc. SPIE*, **6765**, 676504 (2007) (15 pages).
- D2. P.D. Wentzell, "In Profile: Peter D. Wentzell, Dalhousie University", *Analyst*, **128**, 307-308 (2003).
- D1. P.D. Wentzell, "New Approaches to Reaction-Rate Methods of Analysis", *Anal. Proc.*, **26**, 128-130 (1989).

E. Theses Supervised (Dalhousie):

- E15. R.M. Flight, "A Workflow for the Analysis of DNA Microarray Time Course Data", Ph.D. (June, 2009).
- E14. H. Hochreiner, "Modelling Long-Period Fibre Gratings in Chemical Sensing Applications", Ph.D. (January, 2008).
- E13. T.K. Karakach, "Analysis of Gene Expression Data by Multivariate Curve Resolution", Ph.D. (October, 2006).
- E12. L.J. Vega Montoto, "Maximum Likelihood Methods for Three-Way Analysis in Chemistry", Ph.D. (April, 2005).
- E11. M.N. Leger, "Measurement Errors and Signal Preprocessing in Spectroscopy", Ph.D. (September, 2004).
- E10. T.K. Karakach, "Comparison of Linear and Nonlinear Multivariate Calibration Methods", M.Sc. (September, 2002).
- E9. M.N. Leger, "Dynamic Self-Modeling Curve Resolution Method for Multicomponent Mixtures", M.Sc. (August, 2001).
- E8. L.J. Vega-Montoto, "Study of the Performance of Principal Component Regression and Partial Least Squares Regression Using Simulation of Complex Mixtures", M.Sc. (August, 2001).
- E7. C.D. Brown, "Rational Approaches to Data Preprocessing in Multivariate Calibration", Ph.D. (August, 2000).
- E6. M.T. Lohnes, "Multivariate Approaches to Qualitative and Quantitative Analysis in Chemistry: 1. Calibration with Correlated Errors, 2. Window-Target-Testing Factor Analysis", M.Sc. (June, 1998).
- E5. S.A. Mehlman, "Modeling Mixtures in Chemistry: Some Nonlinear Optimization Problems", M.Sc. (December, 1997).

- E4. D.T. Andrews, "Maximum Likelihood Multivariate Methods in Analytical Chemistry", Ph.D. Thesis (May, 1997).
 E3. S.G. Hughes, "Chemometrics for Ordered and Disordered Data Sets", Ph.D. Thesis (December, 1995).
 E2. S.J. Vanslyke, "Enhancements to Multidimensional Methods in Analytical Chemistry", Ph.D. (May, 1994).
 E1. N.G. Sundin, "Automated Mapping of Response Surfaces for Continuous Flow Methods of Analysis", M.Sc. (December, 1991).

F. Presentations:

(* = presenting author, † = invited presentation, ‡ = poster)

- †F137. P.D. Wentzell* and S. Hou, "Exploratory Data Analysis with Noisy Data", Eastern Analytical Symposium, Somerset, NJ, USA, Nov. 16-19, 2009.
- F136. R.M. Flight* and P.D. Wentzell, "Sequential Normalization of Time-Course DNA Microarray Data", Atlantic Computational Life Sciences Challenges Workshop, Sackville, NB, Nov. 14, 2009.
- F135. S.Hou* and P.D. Wentzell, "Dealing with Non-Uniform Measurement Uncertainties: An Application of Maximum Likelihood Methods to DNA Microarray Data", Atlantic Computational Life Sciences Challenges Workshop, Sackville, NB, Nov. 14, 2009.
- F134. R.M. Flight* and P.D. Wentzell, "Normalization Methods for Time-course DNA Microarray Data", Robert Cedergren Bioinformatics Colloquium 2009, Montreal, Quebec, Nov. 5-6, 2009.
- †F133. P.D. Wentzell*, "Measurement Errors in Gene Expression Data from Spotted DNA Microarrays", Lorentz Workshop on Experimental Design in Systems Biology: Data Analysis and Parameter Identification, Leiden, The Netherlands, June 2-5, 2009.
- ‡F132. R.M. Flight* and P.D. Wentzell, "What's in a Workflow? Understanding Time Course DNA Microarray Data Using Multivariate Curve Resolution", Atlantic Omics Symposium, Moncton, NB, Aug. 19-20, 2008.
- ‡F131. J.O. Onochie*, R.M. Flight and P.D. Wentzell, "Investigation of tGene Expression Profiles in *Saccharomyces Cerevisiae* Exiting Stationary Phase", Atlantic Omics Symposium, Moncton, NB, Aug. 19-20, 2008.
- ‡F130. B. Wielens*, R.M. Flight and P.D. Wentzell, "The GENEMACHINE – Software for Gene Expression Analysis", Atlantic Omics Symposium, Moncton, NB, Aug. 19-20, 2008.
- F129. P.D. Wentzell*, R.M. Flight, J.M. Boutilier, B.L. Wielens, and J.O. Onochie, "From Measurement to Knowledge: A Workflow for Multivariate Curve Resolution of DNA Microarray Data", Chemometrics in Analytical Chemistry Conference 2008, Montpellier, France, June 30-July 4, 2008.
- ‡F128. H. Hochreiner* and P.D. Wentzell, "Modelling New Applications of Long-Period Fibre Gratings: Absorbance Measurements," Eurotrode IX, Dublin, Ireland, Mar. 30 – Apr. 2, 2008.
- F127. R. Tauler* and P.D. Wentzell, "Consideration of Measurement Uncertainties in Multivariate Curve Resolution by Alternating Least Squares", FACSS 2007, Memphis, TN, Oct. 12-18, 2007.
- F126. H. Hochreiner*, M. Cada and P.D. Wentzell, "Tuning the Response of Long-Period Fiber Gratings for Chemical Sensing Applications", SPIE Optics East, Boston, MA, Sept. 9-12, 2007.
- ‡F125. J. Boutilier*, R.M. Flight and P.D. Wentzell, "Gridding Reproducibility in Spotted DNA Microarrays", Atlantic Omics Symposium, Moncton, NB, August 22-23, 2007. (2nd place prize in poster competition.)
- F124. P.D. Wentzell*, "DNA Microarrays and the Secret Life of Yeast: An Analytical Approach", Dept. of Chemistry, Cape Breton University, Sydney, NS, Feb. 13, 2007
- †F123. P.D. Wentzell*, "Beautiful Noise: Characterization of Multivariate Measurement Errors", Eastern Analytical Symposium, Somerset, NJ, Nov. 13-16, 2006.
- F122. R.M. Flight* and P.D. Wentzell, "Deciphering the Transcription Patterns of a Malaria Parasite Using Multivariate Curve Resolution", 10th International Conference on Chemometrics in Analytical Chemistry, Águas de Lindóia – SP, Brazil, Sept. 10-15, 2006.
- ‡F121. T.K. Karakach* and P.D. Wentzell, "Characterization of Errors in Transcriptomics by Spotted DNA Microarray Data", 10th International Conference on Chemometrics in Analytical Chemistry, Águas de Lindóia – SP, Brazil, Sept. 10-15, 2006 (winner of Poster Award).
- ‡F120. R.M. Flight* and P.D. Wentzell, "Deciphering the Transcription Patterns of a Malaria Parasite Using Multivariate Curve Resolution", Atlantic Microarray Symposium, Moncton, NB, August 24-25, 2006.
- †F119. P.D. Wentzell*, "Arrays and Microarrays: Chemistry Meets Biology", The Dow Chemical Company, Midland, MI (online seminar presented to 5 remote locations in US and Europe), July 27, 2006.
- F118. H. Hochreiner*, M. Cada and P.D. Wentzell, "Theoretical Considerations in the use of Long-Period Gratings as Chemical Sensors", Canadian Society for Chemistry Conference, Halifax, NS, May 27-31, 2006.
- †F117. P.D. Wentzell*, T.K. Karakach and R.M. Flight, "Watching the Cellular Crockpot: An Analytical Approach to Gene Expression Monitoring with DNA Microarrays", Canadian Society for Chemistry Conference, Halifax, NS, May 27-31, 2006.
- †F116. P.D. Wentzell*, "The Red-Green Show: An Analytical Chemist Looks at DNA Microarrays", University of Prince Edward Island, Charlottetown, PEI, Feb. 24, 2006.

- †F115. P.D. Wentzell, "Recent Developments in Assessing and Utilizing Measurement Error Information in Multivariate Analysis", EAS 2005, Somerset, NJ, Nov. 14-17, 2005.
- †F114. L. Vega Montoto and P.D. Wentzell, "Maximum Likelihood Methods for Three-Way Analysis in Chemistry", FACSS 2005, Quebec City, QC, Oct. 9-13, 2005.
- †F113. P.D. Wentzell, T.K. Karakach and R.N. Flight, "Strategies for the Analysis of Microarray Time Course Data", Atlantic Microarray Symposium, Moncton, NB, Aug. 25, 2005.
- †F112. P.D. Wentzell, "Introduction to DNA Microarray Analysis", Faculty of Computer Science, Dalhousie University, March 21, 2005.
- †F111. P.D. Wentzell, T.K. Karakach, M. Werner-Washburne and M.J. Martinez, "Chemometrics, Microarrays and the Secret Life of Yeast", Chemometrics in Analytical Chemistry Conference 2004, Lisbon, Portugal, Sept. 19-23, 2004.
- ‡F110. T.K. Karakach and P.D. Wentzell, "The Background Phenomenon and Normalization of cDNA Microarray Data", Chemometrics in Analytical Chemistry Conference 2004, Lisbon, Portugal, Sept. 19-23, 2004.
- †F109. P.D. Wentzell, "DNA Microarray Time Course Studies in Yeast", Dept. of Biochemistry and Molecular Biology, Dalhousie University, Halifax, NS, April 22, 2004.
- †F108. P.D. Wentzell, "The Secret Life of Yeast: Chemometrics in the Analysis of DNA Microarrays", Dept. of Chemistry, Dalhousie University, Halifax, NS, Jan. 16, 2004.
- †F107. P.D. Wentzell, T.K. Karakach and M.N. Leger, "Strategies for Multivariate Curve Resolution in the Presence of Non-Uniform Measurement Errors", Eastern Analytical Symposium 2003, Somerset, NJ, Nov. 17-20, 2003.
- †F106. P.D. Wentzell, T. Karakach, M. Werner-Washburne and J. Martinez, "Measurement Error Considerations in the Analysis of DNA Microarray Data", FACSS 2003, Ft. Lauderdale, FL, Oct. 19-23, 2003.
- F105. M.N. Leger and P.D. Wentzell, "Perspectives on Preprocessing in Near Infrared Spectroscopy", FACSS 2003, Ft. Lauderdale, FL, Oct. 19-23, 2003.
- F104. L. Vega-Montoto and P.D. Wentzell, "Incorporating Measurement Error Information into Three-Way Analysis", FACSS 2003, Ft. Lauderdale, FL, Oct. 19-23, 2003.
- ‡F103. P.D. Wentzell and T.K. Karakach, "Estimation of Ratio Measurement Uncertainty in Microarray Data Analysis", Cambridge Health Institute Microarray Data Analysis Conference, Baltimore, MD, Sept. 21-23, 2003.
- †F102. P.D. Wentzell, "Maximum Likelihood Multivariate Calibration", Gordon Research Conference on Statistics in Chemistry and Chemical Engineering, Mt. Holyoke College, South Hadley, MA, July 27-Aug. 1, 2003.
- †F101. P.D. Wentzell, "Some Studies on Spot Morphology and Reproducibility in Yeast Microarrays", Cancer Research and Treatment Center, University of New Mexico, Albuquerque, NM, April 24, 2003.
- †F100. P.D. Wentzell, "Seeing Spots – An Assessment of the Quality of Ratio Data from DNA Microarrays", Department of Chemistry, Arizona State University, Tempe, AZ, March 27, 2003.
- F99. T.K. Karakach and P.D. Wentzell, "Comparison of Nonlinear Multivariate Calibration Methods using UV Absorbance Data from a Designed Experiment", Pittsburgh Conference, Orlando, FL, March 9-14, 2003.
- †F98. P.D. Wentzell, "Analytical Chemistry in Hyperspace: Chemometrics as a Tool for Unravelling Multivariate Data", Department of Chemistry, McGill University, Montreal, Quebec, November 26, 2002.
- F97. L. Vega-Montoto and P.D. Wentzell, "Maximum Likelihood Parallel Factor Analysis (MLPARAFAC)" Chemometrics in Analytical Chemistry (CAC-2002), Seattle, WA, Sept.21-26, 2002.
- ‡F96. M.N. Leger and P.D. Wentzell, "Models for Measurement Error Covariance in Multichannel Instrumentation", Chemometrics in Analytical Chemistry (CAC-2002), Seattle, WA, Sept.21-26, 2002.
- †F94-5. P.D. Wentzell, "Northern Exposure: Chemometrics Research at Dalhousie University", Dept. of Chemistry, University of New Mexico and InLight Solutions Inc., Albuquerque, NM, June 13 and 14, 2002.
- F93. P.D. Wentzell and M.N. Leger, "Dynamic Monte-Carlo Self-Modeling Curve Resolution", Pittsburgh Conference, New Orleans, LA, March 17-22, 2002.
- F92. P.D. Wentzell, M.N. Leger, S.K. Shreyer and M.S. Kemper, "Maximum Likelihood Principal Components Analysis and Data Fusion: Theoretical and Experimental Investigations Using Near Infrared and Raman Spectroscopy", Pittsburgh Conference, New Orleans, LA, March 17-22, 2002.
- †F91. P.D. Wentzell, "Analytical Chemistry in Hyperspace: Chemometrics as a Tool for Unravelling Multivariate Data", Department of Chemistry, University of Toronto, Toronto, ON, Feb. 1, 2002.
- F90. P.D. Wentzell, S.K. Shreyer and M.S. Kemper, "Case Studies in the Application of Maximum Likelihood Principal Components Analysis", 7th Scandinavian Symposium on Chemometrics, Copenhagen, Denmark, Aug. 19-23, 2001.
- †F89. P.D. Wentzell, "Chemometric Vignettes: A Glimpse at Statistics in the World of Chemistry", Dept. of Mathematics and Statistics, Dalhousie University, Halifax, NS, Feb. 8, 2001.
- F88. P.D. Wentzell, "Chemometrics: Analytical Chemistry in Hyperspace", Dept. of Chemistry, University of Prince Edward Island, Charlottetown, PEI, December 1, 2000.
- F87. P.D. Wentzell, "New Paradigms for Chemical Data Analysis (or How Math is Cheaper than Physics)", Dept. of Chemistry, St. Mary's University, Halifax, NS, November 17, 2000.
- F86. P.D. Wentzell, S. Nair and R.D. Guy, "Trilinear Decomposition of Fluorescence Quenching Data for the Identification of Polycyclic Aromatic Hydrocarbons", 7th International Conference on Chemometrics in Analytical Chemistry, Antwerp, Belgium, October 16-20, 2000.

- ‡F85. M.N. Leger[†] and P.D. Wentzell, "A New Approach to Self-Modeling Curve Resolution: Why Lawton and Sylvestre Were Wrong", 7th International Conference on Chemometrics in Analytical Chemistry, Antwerp, Belgium, October 16-20, 2000.
- ‡F84. P.D. Wentzell[†] and C.D. Brown, "Optimal Preprocessing and Maximum Likelihood Principal Components Analysis", 7th International Conference on Chemometrics in Analytical Chemistry, Antwerp, Belgium, October 16-20, 2000.
- †F83. P.D. Wentzell[†], "Unearthing Hidden Treasure in Data with Chemometric Shovels", Dept. of Chemistry, University of Waterloo, Waterloo, ON, August 11, 2000.
- †F82. P.D. Wentzell[†], "The Missing Dimension in Chemometrics", Dept. of Chemistry, University of Ohio, Athens, OH, April 14, 2000.
- F81. P.D. Wentzell[†], S. Nair and M.N. Leger, "Third-Order Data Analysis for the Identification and Quantitation of Polycyclic Aromatic Compounds in Complex Samples by Fluorescence Spectroscopy", Pittsburgh Conference, New Orleans, LA, March 12-17, 2000.
- F80. C.D. Brown[†] and P.D. Wentzell, "Rational Approaches to Preprocessing in Multivariate Calibration", Pittsburgh Conference, New Orleans, LA, March 12-17, 2000.
- F79. P.D. Wentzell[†], "Theoretical Analytical Chemistry", Dept. of Chemistry, University of Victoria, Victoria, BC, October 29, 1999.
- F78. C.D. Brown[†], P.D. Wentzell and L. Vega-Montoto, "Derivative Filters in Multivariate Calibration: Looking Under the Hood", FACSS 1999, Vancouver, BC, October 24-29, 1999.
- †F77. P.D. Wentzell[†] and L. Vega-Montoto, "Rationalizing Multivariate Calibration through Chemical Mixture Models", FACSS 1999, Vancouver, BC, October 24-29, 1999.
- †F76. P.D. Wentzell[†] and C.D. Brown, "Towards Optimal Pre-processing in Multivariate Calibration", Eastern Analytical Symposium, Somerset, New Jersey, Nov. 16-19, 1998.
- †F75. P.D. Wentzell[†], J.H. Wang, L.F. Loucks and K.M. Miller, "A New Approach to Self-Modelling Curve Resolution", Eastern Analytical Symposium, Somerset, New Jersey, Nov. 16-19, 1998.
- †F74. P.D. Wentzell[†], "Applications of Multivariate Methods to Complex Petroleum Samples", FACSS 1998, Austin, Texas, Oct. 12-15, 1998.
- †F73. P.D. Wentzell[†], "Reflections on Maximum Likelihood Multivariate Calibration Methods", FACSS 1998, Austin, Texas, Oct. 12-15, 1998.
- F72. C.D. Brown[†] and P.D. Wentzell, "Hazards of Digital Filtering in Multivariate Calibration", FACSS 1998, Austin, Texas, Oct. 12-15, 1998.
- †F71. P.D. Wentzell[†], "Snap, Crackle, Pop: Acoustic Emission in Chemistry", Union Carbide Corp., Charleston, WV, May 20, 1998.
- †F70. P.D. Wentzell[†], "Measurement Errors in Multivariate Analysis: The Good, the Bad, and the Ugly", First Conference on Chemometrics in China, Zhangjiajie, People's Republic of China, Oct. 17-23, 1997.
- †F69. P.D. Wentzell[†], "Theoretical Analytical Chemistry", Dept. of Chemistry, Dalhousie University, Halifax, NS, Sept. 26, 1997.
- †F66-8. P.D. Wentzell[†], "Acoustic Emission Analysis: Listening to Analytical Chemistry" Invited Lecture Tour sponsored by the Atlantic Provinces Council on the Sciences (APICS), 1997. Universities visited: University of Prince Edward Island (Mar. 7), St. Francis Xavier University (Mar. 12), Acadia University (Mar. 14).
- †F65. P.D. Wentzell[†], "Maximum Likelihood Principal Components Analysis: The Musings of a Chemometrician", Dept. of Mathematics, Statistics and Computer Science, Dalhousie University, Halifax, NS, Oct. 17, 1996.
- †F64. P.D. Wentzell[†], "Some 'Really Neat' Passive Acoustic Sensing Methods", 212th ACS National Meeting, Orlando, FL, Aug. 25-29, 1996.
- †F63. P.D. Wentzell[†], "Chemometrics: New Perspectives on Some Old Ideas", University of Delaware, Newark, DE, Nov. 16, 1995.
- †F62. P.D. Wentzell[†], "Gauss, Darwin and Chemometrics", University of Prince Edward Island, Nov. 2, 1995.
- †F61. P.D. Wentzell[†] and D.T. Andrews, "Regression and Principal Component Analysis: A Unified View", 35th IUPAC Congress, Istanbul, Turkey, August 14-19, 1995.
- ‡F60. P.D. Wentzell[†] and M.J. Little, "An Acoustic Based Method for the Determination of Carbonate", 35th IUPAC Congress, Istanbul, Turkey, August 14-19, 1995.
- ‡F59. P.D. Wentzell[†], S.G. Hughes and S.J. Vanslyke, "Evolving Projection Analysis: A Tool for the Analysis of Multicomponent Mixtures", 35th IUPAC Congress, Istanbul, Turkey, August 14-19, 1995.
- †F58. P.D. Wentzell[†], "Maximum Likelihood Principal Component Analysis", Gordon Research Conference on Statistics in Chemistry and Chemical Engineering, New Hampton, New Hampshire, July 30-Aug. 5, 1995.
- †F57. P.D. Wentzell[†], S.G. Hughes and C.B. Lucasius, "Solving Chemical Problems with Genetic Algorithms", 78th CSC Conference, Guelph, Ontario, May 28-June 1, 1995.
- F56. P.D. Wentzell[†] and S.G. Hughes, "Evolving Projection Analysis of Multicomponent Mixtures", 78th CSC Conference, Guelph, Ontario, May 28-June 1, 1995.
- †F55. P.D. Wentzell[†], M.J. Little, K.B. Thurbide and W.A. Aue, "Novel Methods of Passive Acoustic Sensing for Quantitative Analysis", 78th CSC Conference, Guelph, Ontario, May 28-June 1, 1995.
- F54. D.T. Andrews[†] and P.D. Wentzell, "What is a Principal Component Anyway?", 78th CSC Conference, Guelph, Ontario, May 28-June 1, 1995.

- †F53. P.D. Wentzell, "Chemometric Vignettes: Something Old, Something New, Something Borrowed, and Something To Do", Center for Process Analytical Chemistry/Department of Chemistry, University of Washington, Seattle, WA, Feb. 6, 1995.
- F51-2. P.D. Wentzell, "Chemometrics: Tools for Our Times", Department of Chemistry, Bishop's University, Lennoxville, Quebec, Nov. 9, 1994, and Department of Chemistry, University of New Brunswick, Fredericton, NB, Nov. 14, 1994.
- †F50. P.D. Wentzell, "Parallel Digital Filters for Ordered Spectral Data Sets", Fifth Symposium on Computer-Enhanced Analytical Spectroscopy, Snowbird, Salt Lake City, Utah, June 15-17, 1994.
- F49. P.D. Wentzell*, S.G. Hughes and S.J. Vanslyke, "'Innovations' in Chromatographic Curve Resolution", presented at the 1994 CSC Conference, Winnipeg, Manitoba, May 29-June 2, 1994.
- F48. S.G. Hughes*, P.D. Wentzell, R.F. McCurdy and R.K. Boss "Predicting Conductivity in Non-Brine Water Samples", presented at the 1994 CSC Conference, Winnipeg, Manitoba, May 29-June 2, 1994.
- †F47. P.D. Wentzell*, "Principal Components Analysis: A Common Thread in Chemometrics", Concordia University, Montreal, Quebec, March 25, 1994.
- †F46. P.D. Wentzell*, "Chemometrics: Black Magic of Analytical Chemistry", Mount Allison University, Sackville, NB, November 11, 1993.
- †F45. P.D. Wentzell*, S.G. Hughes and S.J. Vanslyke, "Chromatographic Curve Resolution in the Real World: Nonlinearities and Other Limitations", FACSS 1993, Detroit, MI, Oct. 17-22, 1993.
- F44. P.D. Wentzell*, S.G. Hughes, R.K. Boss and R.F. McCurdy, "Models for Conductance Measurements in the Quality Assurance of Water Analysis", FACSS 1993, Detroit, MI, Oct. 17-22, 1993.
- †F43. P.D. Wentzell*, N.G. Sundin and C. Hogeboom, "Flow-Injection Mapping of Response Surfaces in Hydride Generation Atomic Absorption Spectroscopy", FACSS 1993, Detroit, MI, Oct. 17-22, 1993.
- ‡F42. R.K. Boyd*, M.A. Quilliam, S. Pleasance, S.J. Vanslyke and P.D. Wentzell, "Optimization of the Ionspray Mass Spectrometer as an LC Detector", 41st ASMS Conference on Mass Spectrometry, San Francisco, CA, May 30 - June 4, 1993.
- †F41. P.D. Wentzell*, "Mathematics in Chemistry", Grade 12 Lecture, Halifax Grammar School, Halifax, N.S., February 18, 1993.
- †F40. P.D. Wentzell*, "Acoustics in Chemistry", Meeting of the Canadian Acoustical Association (Halifax Chapter), Halifax, N.S., February 16, 1993.
- †F39. P.D. Wentzell*, "Chemometrics: Black Magic of Analytical Chemistry", Acadia University, Wolfville, N.S., November 12, 1992.
- †F38. P.D. Wentzell*, S.G. Hughes and S.J. Vanslyke, "Digital Filters: They're Not Just for Smoothing Anymore", FACSS 1992, Philadelphia, PA, Sept. 21-25, 1992.
- †F37. P.D. Wentzell*, S.J. Vanslyke and S.G. Hughes, "Real-Time Curve Resolution with the Kalman Filter", Fifth International Conference on Chemometrics in Analytical Chemistry, Montreal, Quebec, July 14-17, 1992.
- ‡F36. P.D. Wentzell*, R.L. White, M.A. Beasy, D.W. Grund and D.S. Clark, "Taxonomy of mushrooms by Pattern Recognition of Chromatographic Data", Fifth International Conference on Chemometrics in Analytical Chemistry, Montreal, Quebec, July 14-17, 1992.
- ‡F35. P.D. Wentzell*, S.J. Vanslyke, and S.G. Hughes, "Spectral Analysis on the Fly: Principal Components Analysis Meets the Kalman Filter", Fourth Symposium on Computer-Enhanced Analytical Spectroscopy, Snowbird, Salt Lake City, Utah, June 17-19, 1992.
- †F34. P.D. Wentzell*, "Chemometric Tools for Solving Analytical Problems", presented at the 11th Annual Meeting of the Association of Official Analytical Chemists (AOAC), Northeast Regional Section, Halifax, NS, May 10-12, 1992.
- F33. S.J. Vanslyke*, P.D. Wentzell, S. Pleasance, and R.K. Boyd, "Optimization of Ionspray Interface Parameters for Combined Liquid Chromatography - Mass Spectrometry", presented at the Pittsburgh Conference in Analytical Chemistry, New Orleans, LA, March 9-13, 1992.
- †F27-32. P.D. Wentzell*, "Chemometrics: Black Magic of Analytical Chemistry", Invited Lecture Tour sponsored by the Atlantic Provinces Council on the Sciences (APICS), 1992. Atlantic universities visited: Dalhousie University (Jan. 31), St. Mary's University (Feb. 7), Memorial University of Newfoundland (Feb. 10), Sir Wilfred Grenfell College (Feb. 11), University College of Cape Breton (Feb. 17), St. Francis Xavier University (Feb. 18).
- †F26. P.D. Wentzell*, M. Bowdridge, and C. MacDonald, "Dispersion in Flow Injection Analysis: The Random Walk Model Revisited", presented at the Winter Conference on Flow Injection Analysis", Scottsdale, AZ, Jan. 12-14, 1992.
- F25. N.G. Sundin* and P.D. Wentzell, "Real-Time Response Surface Modeling for Chemical Systems", presented at the 1991 Canadian Chemical Conference, Hamilton, ON, June 2-7, 1991.
- F24. S.J. Vanslyke* and P.D. Wentzell, "Kalman Filter Networks for Chemical Measurements", presented at the 1991 Canadian Chemical Conference, Hamilton, ON, June 2-7, 1991.
- F23. P.D. Wentzell* and N.G. Sundin, "Automated Real-Time Response Surface Mapping for Continuous Flow Systems", presented at the Pittsburgh Conference and Exposition, Chicago, IL, March 4-8, 1991.
- F22. P.D. Wentzell*, S.J. Vanslyke and K.P. Bateman, "Chemical Analysis by Acoustic Emission", presented at the annual FACSS conference, Cleveland, OH, October 7-12, 1990.
- †F21. P.D. Wentzell* and S.J. Vanslyke, "Application of Digital Filter Networks to Chemical Measurements", presented at the annual FACSS conference, Cleveland, OH, October 7-12, 1990.

- F20. A.P. Wade^{*}, P.M. Shiundu and P.D. Wentzell, "Automated Exploration and Exploitation of Response Surfaces", presented at the annual FACSS conference, Cleveland, OH, October 7-12, 1990.
- F19. P.D. Wentzell^{*} and K.P. Bateman, "Chemical Analysis by Acoustic Emission", presented at the 1990 Canadian Chemical Conference, Halifax, NS, July 15-20, 1990.
- †F18. P.D. Wentzell^{*}, "Chemical Acoustic Emission Analysis: The Sounds of Chemistry", presented at the University of Prince Edward Island, Charlottetown, P.E.I., March 5, 1990.
- F17. A.P. Wade^{*}, S.J. Vanslyke, I.H. Brock and P.D. Wentzell, "Acoustic Emission: On Sampling, Sensors, and Signal Interpretation", presented at the annual FACSS conference, Chicago, IL, October 1-6, 1989.
- F16. P.M. Shiundu^{*}, P.D. Wentzell and A.P. Wade, "Characterization of Sulphochlorophenolazorhodanine as a Reagent for Palladium in Flow Injection Analysis", presented at the annual FACSS conference, Chicago, IL, October 1-6, 1989.
- F15. P.D. Wentzell^{*}, "Solution Robotics: The Chemist's Workbench", presented at the 1989 CIC Conference, Victoria, BC, June 4-8, 1989.
- F14. P.D. Wentzell^{*}, D. Sibbald, D.A. Boyd and A.P. Wade, "Chemometric Methods for Acoustic Emission Analysis", presented at the annual FACSS conference, Boston, MA, October 30-November 4, 1988.
- F13. D.Sibbald^{*}, P.D. Wentzell, D.A. Boyd, O. Lee and A.P. Wade, "Is Acoustic Emission Just Going Through a Phase?", presented at the annual FACSS conference, Boston, MA, October 30-November 4, 1988.
- F12. A.P. Wade^{*}, P.D. Wentzell, P.M. Shiundu and J.A. Horner, "New Uses of Programmable Hardware in Automated Flow Injection Analysis", presented at the annual FACSS conference, Boston, MA, October 30-November 4, 1988.
- F11. P.M. Shiundu^{*}, P.D. Wentzell and A.P. Wade, "Automated Methods Development for Flow Injection Analysis: Some Case Studies", presented at the annual FACSS conference, Boston, MA, October 30-November 4, 1988.
- F10. T.D. Hettipathirana^{*}, M.W. Blades, P.D. Wentzell and A.P. Wade, "Automated Study of the Acetic Acid Interference Effects in ICPOES by Flow Injection Analysis", presented at the annual FACSS conference, Boston, MA, October 30-November 4, 1988.
- F9. P.D. Wentzell^{*}, "New Approaches to Reaction-Rate Methods of Analysis", presented at the Autumn Meeting of the Royal Society of Chemistry, Birmingham, England, September 20-22, 1988.
- F8. A.P. Wade^{*}, P.M. Shiundu, and P.D. Wentzell, "Automated Development of FIA Methods by Adaptive Control", presented at Flow Analysis IV, Las Vegas, Nevada, April 17-20, 1988.
- F7. P.D. Wentzell^{*} and A.P. Wade, "A New Approach to Experimental Optimization: Simplex Meets the Kalman Filter", presented at the Pittsburgh Conference and Exposition, New Orleans, LA, February 22-26, 1988.
- F6. P.D. Wentzell^{*}, A.P. Wade, and S.R. Crouch, "Modeling Response Surfaces with the Kalman Filter", presented at the annual FACSS conference, Detroit, MI, October 4-9, 1987.
- F5. P.D. Wentzell^{*}, S.K. Ratanathanawongs, K. Kurtz, and S.R. Crouch, "Recycling Heartcut Chromatography: Theory and Evaluation", presented at the annual FACSS conference, Detroit, MI, October 4-9, 1987.
- F4. T.P. Doherty^{*}, P.D. Wentzell, and S.R. Crouch, "Interpreting the Frequency Response of Digital Filters", presented at the annual FACSS conference, St. Louis, MO, September 28-October 3, 1986.
- F3. P.D. Wentzell^{*} and S.R. Crouch, "The Kalman Filter for Reaction-Rate Methods of Analysis", presented at the annual FACSS conference, St. Louis, MO, September 28-October 3, 1986.
- F2. S.R. Crouch^{*} and P.D. Wentzell, "New Data Handling Methods for Reaction-Rate Determinations", presented at the Second International Symposium on Kinetics in Analytical Chemistry, Preveza, Greece, September 9-12, 1986.
- ‡F1. P.D. Wentzell^{*} and S.R. Crouch, "A Reaction-Rate Method Insensitive to Changes in the Rate Constant", presented at the annual conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS), Philadelphia, PA, September 29-October 4, 1985.