Chemistry Department
Annual Report
Period: July 1, 2003 – June 30, 2004

Fiscal year 2004 was a momentous period for the Department of Chemistry. Many traditions begun during the past six years were continued such as (1) publication of the semi-annual alumni magazine, ELEMENTS, in October and April; (2) meeting of the department's Advisory Council in September and April; (3) Student Awards Ceremony in May; (4) two faculty-alumni banquets in the Fall and Spring; (5) the summer faculty-staff picnic; (6) secretary's lunch with the faculty in April; (7) selection of the Clifford Faculty Service Award, the McNair Staff Service Award, the Gary Cook Faculty Research Award, the Gary Cook Faculty Teaching Award; and (8) the annual solicitation of monies from the faculty to provide a Christmas gift to all custodians and secretaries.

Several new or less predictable events transpired in FY04. The Department relocated all of its undergraduate laboratory teaching to the new Chemistry/Physics building. All upper division laboratories were held in ChemP Spring 2004. In spite of the noisy ventilation system that has yet to be remedied, the new 50,000 square foot structure and approximately $1.4M in equipment enhanced the quality of instruction greatly.

The Department was also given permission to search for new faculty for the first time in three years. Official searches were conducted in two designated cluster areas: Computational Science and Nano/bioscience. Diego Troya, Research Associate at Northwestern University, accepted the Computational Chemistry position effective July 1, 2004. Two faculty offers were extended in the Nano/bioscience area but they were not accepted. An equally viable third candidate as deemed by the Department faculty was not offered the position. During the academic year, the Department received an application from Yuan-Ping Pang, an outstanding computation/synthetic organic chemistry from the Mayo Clinic in Rochester, MN. An offer of full professor with tenure was given to Pang after a second visit to campus in late February. In late May, the Department was notified by Professor Pang that he could not accept the attractive offer.

The chemistry faculty continues to be recognized for their achievements. Emeritus Professor Harold McNair was selected to be the recipient of the 2004 Award for Achievements in the Fields of Analytical Chemistry by the Governing Board of the Eastern Analytical Symposium, Inc. Professors McGrath and Ward and Professor Wilkes in Chemical Engineering won the Flory Award given by the American Chemical Society Polymer Division for their outstanding teaching of polymer related short courses. Professor Taylor was selected for induction into the Thomas Green Academy of Engineers and Scientist at Clemson University. On campus awardees in the report period from the Chemistry Department include: Gary Long/Barbara Bunn – Alumni Outreach Award; Harry Gibson – Alumni Award for Research Excellence; Hervé Marand/Ketan Trivedi – Xcalibur Award for Achievement in Teaching Technology; and Mark Anderson – Certificate for Teaching Excellence in the College of Science.

The Department is particularly blessed by having two IGERT proposals funded. Professor Riffle is directing one grant aimed at our interdisciplinary degree program in Macromolecular Science and Engineering. The second one co-directed by Professor Tim Long is entitled "Macromolecular Interfaces with Life Sciences." Both grants will result in approximately 40 graduate student fellowship awards per each over a five year period. Other significant grantees: Professor John Morris was the sole awardee of a DURIP grant from Virginia Tech. Daniel Crawford was selected to receive a Cottrell Scholar Award from the Research Corporation. Harry Dorn received a Nanotechnology Undergraduate Education Award aimed at involving college faculty in two hands-on short courses per year.

Outreach by the Department of Chemistry into all regions of the State has been highly effective through the Mobile Chemistry Laboratory and ChemKit programs directed by Professor Gary Long with the aid of Dr. Barbara Bunn. The primary service area of the Mobile Chemistry Laboratory is Southwestern Virginia, Southside Virginia, and inner city Richmond. The ChemKit program serves the entire Commonwealth. Data are kept in terms of Student Conducted Experiments (SCE). For Fall 2003 there were 4,980 MCL SCE at 42 schools and 3,500 ChemKit SCE at 33 schools. In a seven semester period, 43,912 SCE were provided by the Chemistry Outreach Program. This number represents ~ 8,500 students that used the program on a regular basis. Sixty plus teachers have been trained in five basic workshops since 2001 and 39 teachers have been trained in advanced worships since 2002. The average pass rate of the 44 participating high schools is above the state average. Two inner city schools report increases of 70+ points. The schools that have used the MCL for 3+ years have an increase of 37 points, while the state average has risen only 18 points. Funding of the MCL for FY05 was deemed to be unavailable by the Provost and College of Science. Thus, the very successful Chemistry Department outreach project will be discontinued.

The Department continued to operate effectively in FY04 albeit with severe, insufficient financial resources. Five cost recovery service centers in the Department now experience much better management thanks to Professor Hanson. Operation in the "red" should be a "thing of the past". The attached Table captures a fraction of the problem in so far as operation of the Department is concerned. The approximate annual expenditures for FY04 are projected to be $548,179. The allocation to the Department of Chemistry by the University for operation in FY04 was $335,000. Indirect cost recovery by the Department from grants is thus making up a greater part of the difference. Another look at the Table reveals what is needed by the Department on an annual basis to achieve excellence, $700,200. If top 30 status is to be achieved by the Department, "gap funding" cannot be the norm.

While the number of endowments to the Educational Foundation continues to slowly rise in the Department, these funds should not be used for normal operations. The data effective March 2004 are shown in Table 2.

The Department enjoyed another relatively strong year in "generated research dollars". Table 3 compares similar data for Chemistry and other units for FY03 and FY04 (March). On a dollars per faculty basis Chemistry ranks very near the top. Even though the Department has heavily invested in its young faculty and this strategy continued to create significant debt in the manner of two loans, the investment (e.g. start up funds) has paid handsome dividends. See Table 4 for data on the last eight chemistry faculty hires. Each person has already brought in more grant dollars than the University invested in them. The average return per faculty is over 100% per year!

Throughout the past three years, the Department has attempted to meet all its obligations in teaching, research, and outreach in spite of severe budgetary restrictions. The outreach program has been "second to none". The graduate program in terms of enrolled graduate students and research funding has actually increased approximately 20%. The number of weighted student credit hours taught by the Chemistry faculty has actually increased during the last three years. See Table 5 for a comparison of WSCH per allocated faculty position for the past seven years in the Departments of Biology and Chemistry. Chemistry's numbers reflect the situation that existed in 1997. Biology shows a drop of nearly 30%. Service Student Credit Hours continue to be greater than 80% in the Department of Chemistry. Yet, the number of students graduating with an undergraduate degree in Chemistry has remained essentially steady at approximately 50. The same can be said for the granting of advanced degrees in Chemistry (e.g. near 20 each year for the past seven academic years). The Department of Chemistry takes great pride in all of its three functions. The faculty are excellent and highly committed to the University as evidenced by the fact that there has been no attrition to other Universities during the past 10 years. Hopefully, the University will recognize first the excellence that exists in Chemistry by providing additional resources to operate and second demonstrate confidence in the faculty decision making ability that the Department has exhibited for the past ten years.

Table 1
Chemistry Data Revised 4/7/04

Category	Approx. Annual Expenditure	Estimated Need for Excellence
Office Supplies	6,762	7,000
Telecommunications & Ethernet	102,056	114,000
Equipment (New or Replacement)	16,866	20,000
Software	7,473	3,000
Postal & Messenger Services	8,389	7,200
Printing (Courses, Newsletters, etc.)	4,103	19,000
Copier Rental or Purchase & Maint.	14,745	12,000
Equipment Maintenance	35,695	24,000
Shop Supplies and Maint.	5,361	11,000
Catering	1,200	2,000
Tuition & Other Training	-	-
Physical Plant	66,063	112,000
Membership Dues	180	1,000
Travel		
Faculty	17,461	12,000
Grad Students	-	-
Colloquia/Seminars	17,167	11,000
Course/Field Related	771	83,000
Grad and Undergrad Recruiting	17,984	25,000
Wage Employees	39,640	51,000
Labs – Freshman	13,435	14,000
Upper level	61,608	62,000
Lec Prep	2,900	3,000
Other	72,078	70,000
Miscellaneous	36,242	37,000
Total	**548,179**	**700,200**

Table 2
Endowments[a]
Department of Chemistry
March 2004

Hopper Harvie Endowment - $25,911

Chemistry Friends Scholarship - $91,338

Keyser Chemistry Endowment - $28,846

Walker Scholarship - $27,818

Bilisoly Scholarship - $108,540

McNair Fund Endowment - $8,273

Dallas Kinser and R. T. Johnson - $29,161

McGrath Professorship Endowment - $9,300

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[a]J. P. Wightman Scholarship - $33,939
John Dillard Scholarship - $16,252
(Administered by Center for Adhesive and Sealant Science)

Table 3
Generated Research Dollars

	FY 2003	FY 2004 (March)
Dept. Name	Actual Amount	Actual Amt.
Virginia Tech Transportation Instit	$10,496,569	$7,533,753
Dean – Engineering (Power Electronic Center)	$8,984,326	$7,606,903
Electrical Engineering	$8,726,783	$7,864,033
Civil & Envirnomental Engineering	$6,690,307	$5,739,246
Chemistry	$6,198,401	$4,885,767
Mechanical Engineering	$5,482,664	$4,339,436
Virginia Bioinformatics Institute	$4,899,078	$6,103,943
International Res. Edu & Dev	$4,736,730	$3,418,226
Engineering Science & Mechanics	$3,989,430	$2,946,266
Biology	$3,623,554	-

Table 4

INVESTMENT IN CHEMISTRY PAYS-OFF

Grants & Contracts Received

Source: http://dolomite.rgs.vt.edu/webrep/Awards/AwardsMenu

Name	**FY00**	**FY01**	**FY02**	**FY03**	**FY04 April 1**
Ducker	535,000	128,772	347,326	495,000	100,000
Long, T.	413,307	81,801	193,560	1,342,991	754,777
Esker	30,000	15,000	18,500	165,500	375,000
Morris	30,000	709,545	60,000	209,793	250,000
Etzkorn		313, 769	585,565	179,154	-
Carlier		29,600	-	209,000	80,000
Crawford		105,000	157,000	503,000	60,000
Yee			-	320,303	-

Name	**Total Grants FY00-FY04**	**Start-up**	**Residency (years)**
Ducker	1,606,098	254,000	7
Long, T.	2,786,436	204,000	6
Esker	604,000	249,000	5
Morris	1,259,338	274,000	5
Etzkorn	1,078,488	350,000	4
Carlier	318,600	186,000	4
Crawford	825,000	152,000	4
Yee	320,303	252,000	3

Table 5
Teaching and Function

Total Weighted Student Credit Hours (Fall Term)

	1996	**1997**	**1998**	**1999**	**2000**	**2001**	**2002**	**2003**
Chemistry	22,046	20,924	20,770	19,336	19,413	20,367	20,482	21,759
Biology	25,485	24,405	23,133	22,945	21,842	21,505	20,066	18,964

Weighted Student Credit Hours per Allocated Faculty Position

	1996	**1997**	**1998**	**1991**	**2000**	**2001**	**2002**
Chemistry	668	627	567	519	579	590	611
Biology	607	608	536	556	520	512	478

Service Student Credit Hours

	Fall 2001		**Spring 2002**		**Annual Percent Service**
	Major	Non-major	Major	Non-major	
Chemistry	1837	14,362	1828	9701	86.8
Biology	6454	9635	4885	8667	61.7

Primary and Secondary Majors

	97-98	**98-99**	**99-00**	**00-01**	**01-02**	**02-03**	**03-04**
Chemistry (BS/BA)	43 + 11	45 + 5	40 + 14	36 + 11	25 + 5	33 + 11	32 + 15
MS/MA	7	9	6	7	12	6	7
Ph.D.	14	14	16	11	13	12	13

The Planning Domains of Virginia Tech, 2001 and Beyond

Research and Scholarship:

- Professor Gibson – 10 papers published during the period (five in J. Amer. Chem. Soc.), two patent disclosures – one patent application, seven grants funded and in force, five proposals pending
- Professor Dorn – Member of Steering Committee: Initiative for Nanotechnology in VA
- Professor Carlier – five invited lectures off campus – brief write-up in Chemical & Engineering News
- Professor Crawford – "Advanced Quantum Mechanical Methods for Metalloenzymes," Camille and Henry Dreyfus New Faculty Award, $40,000, 09/01-08/04, sole PI; "Accurate Quantum Chemical Methods for Large Molecules," Jeffress Memorial Trust, $40,000, 03/01-03/03, sole PI; "Scalable Fault-Tolerant Algorithms for Linear-Scaling Coupled Cluster Electronic Structure Methods," Department of Energy (Sandia National Laboratories), $180,000, 09/01-09/04, sole PI. Renew and extended by $60,000, 09/03-09/04; "Accurate Quantum Chemical Methods for the Chiropitical Properties of Large Molecules," National Science Foundation CAREER Award, $435,000, 02/02-01/07, sole PI; "Quantum Mechanical Studies of Chirality: Local Correlation Methods for Optical Rotation in Large Molecule," Research Corporation Cottrell Scholar Award, $75,000, 05/03-05/08, sole PI.
- Professor Esker – NSF CAREER Award – Air Force grant
- Professor Morris – NSF CAREER Award "Reaction Dynamics of Hydrogen Halides on OH-Functionalized Surfaces and Development of Guided-Inquiry Experiments for Analytical Chemistry," Level of Responsibility: 100% $502,000; Army Research Office: Young Investigator Award, "Mechanistic Studies of Sarin, VX, and HD Decomposition at the Gas-Surface Interface," Level of Responsibility: 100% $150,000; Army Research Office, "Technical Review of Rebreather Technologies," Level of Responsibility: 100% $50,000; Department of Defense: DURIP Award "Reactions of Chemical Warfare Agent Simulants on Model Polyurethane and Metal-Oxide Surfaces," Level of Responsibility: 100% $109,000
- Professor Kingston – 16 papers published, 11 additional papers submitted for publication, four invited lectures, 13 contributed presentations
- Professor T. Long – total dollars of 2003 grants equals $1,842,700; Department of Chemistry Faculty Research Award; IGERT with Food Science Multiuniversity Research Initiative Grant; Vice-Chair, ACS Division of Polymer Chemistry; Chair, ACS POLY Polymer Design Using Non-Covalent Methods Symposium, 225th ACS National Meeting, New Orleans, LA; Chair, ACS POLY International Workshop on Branched Polymers for Performance, Williamsburg, VA
- Professor Castagnoli – 16 invited lectures worldwide
- Professor McGrath – 14 research papers published or submitted during 2003, one patent received, seven active research grants, five proposals pending, 12 invited lectures to universities and government labs

- Professor Ducker – 11 papers published or submitted for publication, four active federally funded grants, three invited lectures
- Professor Hanson – active in high pressure X-ray crystallography

Graduate Education:

- Professor T. Long – introduced new course with F. Etzkorn entitled "Green Chemistry"
- Professor Riffle – coordinated Interdepartmental Macromolecular Science and Engineering graduate program; Director of IGERT Program, "Macromolecular Science and Infrastructure Engineering"
- Professor Merola – member of committee which writes graduate record examinations

Undergraduate Education:

- Professors Trivedi and Marand - co-authored General Chemistry on DVD
- Professor Ward – winner of the Paul J. Flory Education Award from the Polymer Division of the American Chemical Society (shared with J. E. McGrath and G. L. Wilkes)
- Professor Ward – National Science Foundation REU "Adhesion Science at Virginia Tech"; this new REU began in 2003 and will be ~$150,000
- Professor Amateis – Teaching-Learning Grant from CEUT with Professor Yee "Enhancing Student Success"
- Professor Trivedi – used interactive multimedia DVD as a textbook with great success
- Professor Anderson – Department of Chemistry Faculty Teaching Award; College of Science Certificate of Teaching Excellence; NSF grant (program director) – "REU for Undergraduates in Chemistry at Virginia Tech"
- Professor Crawford – developed "Computational Experiments" for General Chemistry Laboratory entitled "Molecular Modeling and Molecular Structure"
- Professor Esker – John R. Hottle, undergraduate researcher, was the recipient of a $8,500 Virginia Space Grant Consortium Aerospace Undergraduate Research Scholarship for the 2003-2004 Academic Year to carry out research on Polyhedral Oligomeric Silsesquioxane (POSS) and Polymer Blends for Aerospace Applications

Outreach:

- Professor Ward: Primary instructor in each of the following six-day short courses at Virginia Tech: American Chemical Society (ACS) "Principles and Practice of Polymers"; ACS "High Performance Polymeric Adhesives and Composites"; ACS "Principles and Practice of Polymer Chemistry"; "Adhesion Science," June 2003, The Adhesive and Sealant Council sponsored course.
- Mrs. Eddleton – presentation during Parent's weekend: "The Chemistry is Right"
- Professor Bunn – Summer 2003, teacher workshops were held in which the teachers learn how to use the MCL, develop new experiments, etc.

- Professor Brewer – organizer and presenter of Kipps Science Club; Chemistry presentation at Blacksburg Middle School; Chemistry presentation for Kipps Elementary; judge for Blue Ridge Highlands Science Fair
- Professor G. Long – NSF-CHE - Chemistry Outreach to Secondary Schools with a Mobile Chemistry Laboratory, $300,000, September 1, 2001 – August 30, 2004; The Camille and Henry Dreyfus Foundation; Creating Educational Partnerships with Local Industry and Local School Systems via the Mobile Chemistry Laboratory of Virginia Tech, $25,000; DuPont – Support for Traveling Teacher on Mobile Chemistry Laboratory, $25,000, September 1, 2002 to August 30, 2004
- Professor Kingston - 10th Annual meeting of the Suriname-Madagascar International Cooperative biodiversity Group, Paramaribo, Suriname. This meeting was the final one of the Suriname portion of the ICBG program, and included a formal meeting with Government officials and with tribal leaders. International Conference on Biodiversity and Bioactive Compounds, Bio, Thailand 2003, Pattaya, Thailand
- Professor Dillard – Member of the Adhesion Society Executive Committee
- Professor Tanko – elected Vice-Chair of the 2005 Gordon Research Conference on Free Radical Reactions, and Chair of the 2007 Conference.
- Professor Castagnoli – Member, Board of Directors, Edward Via Virginia College of Osteopathic Medicine
- Professor McGrath – Member, Advisory Board for the Center for Advanced Engineering Fibers and Films, Clemson University, Clemson, SC; Member, Advisory Board, University of Illinois NSF Science and Technology Center; Review Board: Navy Research Laboratory Dept. of Chemistry, Sandia National Laboratories Materials Science and Technology, Army Research Office; President, Pacific Polymer Federation, 2003-2005.
- Professor Riffle – ACS Division of Polymer Chemistry: Executive committee member in charge of business office activities

Annual Statistical Information:

Summary of Research and Related Scholarly Activities

Articles in Refereed Journals	98
Presentations at Professional Meetings	30
*Invited Lectures (Off-campus)	108
Research Funding	7.7 million
Books and Monographs	3
Patents	4
Review Articles and Book Chapters	20
Memberships on Journal Editorial Boards	11
Memberships on National Committees	7
Short Courses Taught	13
Students pursued Masters & Ph.D. degrees in 2003-2004 academic year	127
Students received Ph.D. degrees during the 2003-2004 academic year	11
Students received M.S. degrees during the 2003-2004 academic year	7
Students received BA/BS degrees during the 2003-2004 academic year	47

*Does not include invited presentations at professional meetings, which are included in the previous category.