CHEMICAL ENGINEERING GRADUATE PROGRAM

Department of Chemical Engineering
Brigham Young University

THE GRADUATE PROGRAM The Chemical Engineering Department at BYU conducts programs of graduate study leading to master of science (MS) and doctor of philosophy (PhD) degrees. We invite all motivated students to consider expanding their education, understanding, and research skills in our department. Both degrees are research oriented, requiring an original thesis. The focus of the program is on development of the student's ability to conduct independent, creative, scientific research. Graduate students are expected to assume a major responsibility for their own progress and to develop habits of inquiry that will ensure continuing intellectual development throughout their careers. Emphasis is generally placed first on a full understanding of the principles of math, engineering, and science, and then on the application of those principles to present-day engineering problems.

Each member of the faculty is involved in a specific area of graduate level scholarship and research. Research topics vary widely and include such areas as biomedical engineering, catalysis, combustion, electrochemical engineering, environmental engineering, reservoir engineering, teaching pedagogy, and thermodynamics. In addition, most faculty are involved in collaborative and cooperative research—within and beyond department boundaries—some of which is described on this and the next page.

ACERC Combustion research at Brigham Young University is coordinated through the Advanced Combustion Engineering Research Center (ACERC). ACERC is an internationally respected and one of the largest, most productive academic organizations in applied energy research. ACERC is a vertically integrated center, including fundamental research, bench- and pilot-scale laboratory experimentation, full-scale field testing, advanced computational modeling, and solutions to combustion-related problems—all to improve technology through application of fundamental understanding.

Combustion research is currently being conducted on coal, biomass (sawdust, straw, etc.), black liquor (from the papermaking process), petroleum coke, soot formation, and rocket propellants. Previous research has led to new discoveries in fuel reaction processes and rates, methods of acid rain control via NO_x reduction, turbulent reacting flows, fuel minerals behavior, and waste-conversion processes. Highly instrumented lab-scale and pilot-scale reactor facilities allow industrial and academic researchers to characterize the combustion of fuels and wastes in moderate- and high-temperature furnaces, high-intensity (gas turbine) combustors, and exhaust simulation experiments at a variety of scales and pressures that simulate industrial conditions. ACERC strengths include combined computational and experimental research to solve industrial problems such as reducing pollutant emissions, increasing efficiency, and increasing reliability.

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FACULTY:

Calvin Bartholomew
- *Catalysis and Kinetics*

Larry Baxter
- *Catalysis and Kinetics, Combustion, Thermodynamics and Transport Properties, Computing Simulation and Modeling, Environmental Engineering*

Merrill Beckstead
- *Combustion, Chemical Propulsion, Polymers and Composite Materials, Computer Simulation and Modeling*

Thomas Fletcher
- *Combustion, Computer Simulation and Modeling*

Hugh Hales
- *Computer Simulation and Modeling*

John Harb
- *Computer Simulation and Modeling*

William Hecker
- *Catalysis and Kinetics*

John Oscarson
- *Thermodynamics and Transport Properties*

William Pitt
- *Biomedical Materials Engineering*

Richard Rowley
- *Thermodynamics and Transport Properties, Computer Simulation and Modeling*

Kenneth Solen
- *Biomedical Materials Engineering*

Ronald Terry
- *Engineering Pedagogy*

Dean Wheeler
- *Electrochemical Engineering, Computer Simulation and Modeling*

Vincent Wilding (Chair)
- *Environmental Engineering*

THERMOPHYSICAL PROPERTIES LABORATORY (DIPPR-TPL)

Research in the BYU Thermophysical Properties Laboratory involves all aspects of thermophysical properties, but the central effort of TPL involves the DIPPR 801 pure-component evaluated database.

DIPPR, the Design Institute for Physical Properties, is a consortium of chemical process industry companies that funds joint thermophysical property projects under the auspices of AIChE (American Institute of Chemical Engineers). Graduate research projects are focused on two key areas. The first area is the development of new property prediction methods and evaluation of existing prediction methods, which are critical to expanding the database to a variety of new compounds. The second focus is on improving the database by reviewing families and groups of similar compounds to identify the best property values.

Experimental measurements of a variety of thermodynamic and transport properties are made to support process design and development. Among the properties that are measured are heats of reaction, vapor pressures, vapor-liquid equilibrium, vapor and liquid thermal conductivity, liquid density, surface tension, and melting point.

Modern molecular simulation techniques (molecular dynamics and Monte Carlo) are being used to study condensed-phase properties. Molecular simulations are used to understand the molecular underpinnings of thermophysical properties and to predict property values from molecular interactions.

BIOMEDICAL ENGINEERING Biomedical engineering is a broad field encompassing several traditional engineering disciplines, including chemical engineering, mechanical engineering, electrical engineering, and materials science. Professionals from each field contribute in their own ways, given their own particular training.

Because biomedical engineering is one important application of chemical engineering, we provide the opportunity for our students to focus somewhat on this area. The Chemical Engineering Department offers a course on biomedical engineering principles, and we have our students take additional courses in zoology, cell biology, and microbiology to prepare them to conduct research and pursue a career in biomedical engineering.

Two professors in the Department of Chemical Engineering conduct research and teach in the area of biomedical engineering. They are Drs. Ken Solen and Bill Pitt. They have labs and research equipment in our department, but they also collaborate extensively with other research groups in other departments at BYU and elsewhere. A short description of their research efforts can be found in the faculty section of this brochure.

MISSION: The Department of Chemical Engineering exists to support the mission of BYU by preparing students for

- lives of scholarship and continued learning founded upon principles of science, engineering, and mathematics;
- lives of service to family as educated parents, to church as faithful Latter-day Saints, and to community as moral, disciplined, practicing engineers and leaders; and
- lives of contribution to society and humanity by producing products, processes, and policies that improve the quality of life.

Our curriculum is designed to help our students develop the capability to solve problems using both quantitative and non-quantitative information and to communicate the solutions effectively. Our personal interaction with the students is to teach them faith, charity, and respect as a basis for a strong testimony of Jesus Christ and a life consistent with that testimony. Finally, our mission is to accomplish these objectives with effectiveness that is far ahead of the world educationally and spiritually—or, in essence, at the level of a relative Mount Everest.

Calvin H. Bartholomew, Professor (1973–present). PhD and MS, Stanford University (1970 and 1972). BES, Brigham Young University (1968). Head of Catalysis Lab (1973–present).

RESEARCH ACTIVITIES OF PROFESSOR CALVIN H. BARTHOLOMEW

Professor Bartholomew's research focuses on heterogeneous catalysis. Recent projects include the investigation of advanced iron FT catalysts for converting biomass- or coal-derived syngas to gasoline and diesel fuel in collaboration with the University of New Mexico and Texas A&M University. Effects of catalyst composition and pretreatment on the micro-/nano-structures of iron-bimetallic FT catalysts are being investigated using Mössbauer spectroscopy and TEM. Lab reactor tests indicate that Fe-Pt supported on silica is very active and selective for production of FTS hydrocarbon liquids. Moreover, this catalyst promises to be more mechanically stable than conventional iron catalysts.

Study of the kinetics of FTS on cobalt catalysts under commercially relevant conditions is ongoing. These kinetic data are valuable in modeling this process in large FT plants currently under planning or construction in several regions of the world where stranded natural gas is converted to high-grade diesel fuel and fuel oil. Two related projects involve the study of (1) the hydrothermal stability of silica and modified-silica supports in high-pressure steam and (2) methods for coating silica on multicellular ceramic monoliths. In the latter project a method for testing the stability of monolith coatings at high gas flows is being developed. Investigation of the deactivation of SCR catalysts by fly ash minerals in collaboration with Professors Baxter and Hecker of BYU is underway. The study focuses on the poisoning of vanadia/titania catalysts by calcium, potassium, and sodium minerals from coal and biomass.

Student preparing a sample of TGA analysis in the BYU catalysis lab.

PUBLICATIONS

C. H. Bartholomew and R. J. Farrauto, *Fundamentals of Industrial Catalytic Processes,* John-Wiley (2003).

C. H. Bartholomew, "Catalysis Deactivation and Regeneration," *Encyclopedia of Catalysis,* I. T. Horvath (ed.), John-Wiley (2002).

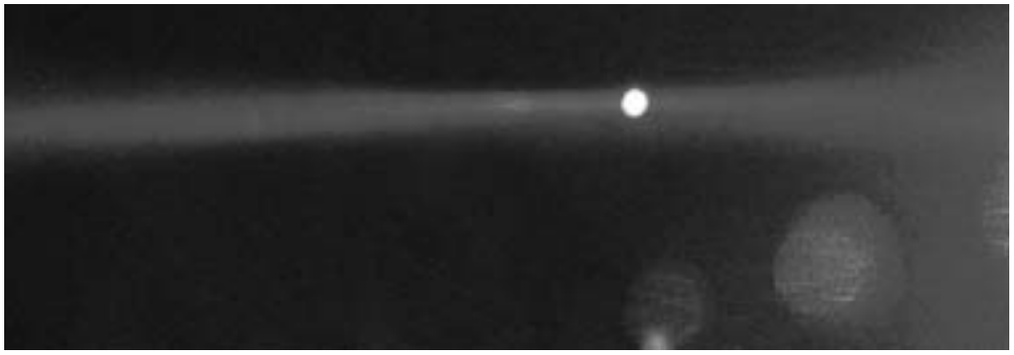
C. H. Bartholomew, "Mechanisms of Catalyst Deactivation," *Applied Catalyst A,* **212,** 17–60 (2001).

G. W. Huber and C. H. Bartholomew, "Pt-Promotion of Co/SiO_2 Fischer-Tropsch Synthesis Catalysts," *Stud. Surf. Sci. & Catal.,* **139,** 283–288 (2001).

Larry L. Baxter, Professor (2000–present). PhD and BS, Brigham Young University (1983 and 1989).

RESEARCH ACTIVITIES OF PROFESSOR LARRY L. BAXTER

The focus of Dr. Baxter's research is the impact of fuel impurities on fuel conversion processes. Specific examples of this work include reduction of pollutant and global warming emissions from power plants, improvements in efficiency and availability of fuel conversion systems, behavior of inorganic material in fuel conversion systems, and development of advanced power generation systems. Dr. Baxter has established research programs on biomass, black liquor, coal, and specialty fuels. Experimental work includes fundamental analyses of individual particles and drops, flow reactor investigations of dynamic combustion processes, pilot-scale work, and fieldwork. Theoretical and modeling work include engineering model development, computer-application-quality programs, and computational fluid mechanics simulations describing reacting, multiphase flows. Current research projects involve specific, formal collaborations with academic and industrial institutions in Denmark, Canada, Finland, Sweden, Germany, Australia, and several institutions in the U.S. Recent contributions by the group include analyzing catalyst deactivation mechanisms associated with low-rank coal and biomass, describing small particle formation and deposition in combustors and gasifiers, developing new experimental techniques for single-particle combustion analyses, and determining corrosion mechanism for chlorine-laden fuels. Dr. Baxter's research goal is to provide information and tools of immediate use and enduring value to practitioners and scientists.



Black liquor fuel particle suspended by an AR+ laser beam.

PUBLICATIONS

A. L. Robinson, H. Junker, L. L. Baxter, et al., "Pilot-scale Investigation of the Influence of Coal-biomass Cofiring on Ash Deposition," *Energy & Fuels*, **16** (2), 343–355 (2002).

A. L. Robinson, S. G. Buckley, L. L. Baxter, et al., "Thermal Conductivity of Ash Deposits 1: Measurement Technique," *Energy & Fuels*, **15,** 66–74 (2001).

A. L. Robinson, S. G. Buckley, L. L. Baxter, et al., "Thermal Conductivity of Ash Deposits 2: Effects of Sintering," *Energy & Fuels*, **15,** 75–84 (2001).

S. Q. Turn, C. M. Kinoshita, L. L. Baxter, et al., "Fuel Characteristics of Processed, High-fiber Sugar Cane," *Fuel Processing Technology* (2001).

R. A. Wessell and L. L. Baxter, "Comprehensive Model of Alkali Salt Deposition in Recovery Boilers," *Tappi Journal* (2001).

L. D. Smoot and L. L. Baxter, "Fossil Fuel Power Stations—Coal Utilization," *Encyclopedia of Physical Science and Technology (*2001).

Merrill W. Beckstead, Professor (1977–present). PhD and BS, University of Utah (1965 and 1961).

RESEARCH ACTIVITIES OF PROFESSOR MERRILL W. BECKSTEAD

Dr. Beckstead's research group focuses on combustion-related projects with specific application to solid propellants. The group investigates and models different phases of stable, unstable, and transient combustion. It has developed theoretical models to describe the steady-state combustion of all varieties of solid propellants in use today and has performed fundamental work on diffusion flames applying to solid propellant configurations.

Current emphasis has been on integrating large kinetic mechanisms into basic models of propellant ingredients. Dr. Beckstead's group has developed a state-of-the-art model that predicts various combustion characteristics for the more common propellant ingredients. This approach has also been applied to unsteady combustion, describing the detailed combustion instability characteristics that can occur in solid propellants.

During the past decade two models have been developed to describe the combustion of metal particles with emphasis on aluminum combustion.

Trident missile launch from a submarine.

PUBLICATIONS

M. W. Beckstead, B. R. Newbold, and C. Waroquet, "A Summary of Aluminum Combustion," *Proceedings of the Thirty-Seventh JANNAF Combustion Meeting,* Monterey, California, November 2000, CPIA, **701,** no.1, 485–504 (2000).

M. W. Beckstead, "An Overview of Combustion Mechanisms and Flame Structure of Advanced Solid Propellants," *Solid Propellant Chemistry Combustion and Motor Interior Ballistics,* **185,** 267–286 (2000).

J. E. Davidson and M. W. Beckstead, "Improvements to RDX Combustion Modeling," *Journal of Propulsion and Power,* **13,** no. 3, 375–383 (1997).

F. S. Blomshield, H. B. Mathes, J. E. Crump, C. A. Beiter, and M. W. Beckstead, "Nonlinear Stability Testing and Pulsing of Full-scale Tactical Motors," *Journal of Propulsion and Power,* **13,** no. 3, 356–366 (1997).

M. W. Beckstead and J. E. Davidson, and Q. Jing, "A Comparison of Solid Monopropellant Combustion and Modeling," *The Fourth International Symposium on Special Topics in Chemical Propulsion,* Stockholm, Sweden (1996).

J. E. Davidson and M. W. Beckstead, "A Three-Phase Model of HMX Combustion," *The Proceedings of the Twenty-Sixth International Symposium on Combustion,* The Combustion Institute (1989–1996).

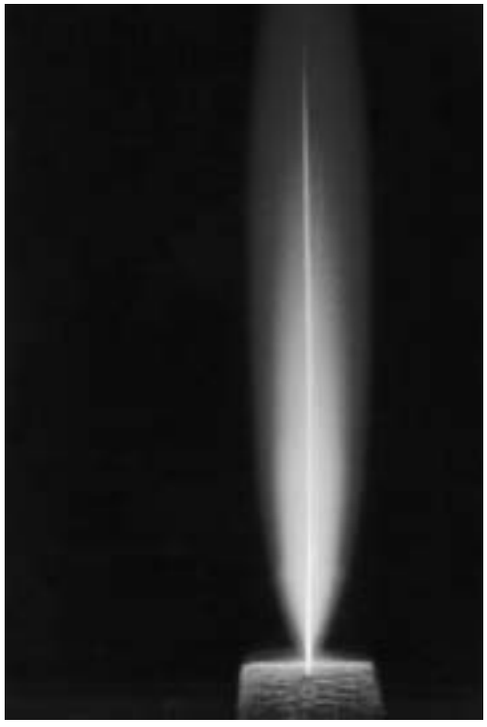
Thomas H. Fletcher, Professor (1991–present). PhD, MS, and BS, Brigham Young University (1983, 1980, and 1979). Director, Advanced Combustion Engineering Research Center (1997–present).

RESEARCH ACTIVITIES OF PROFESSOR THOMAS H. FLETCHER

Dr. Fletcher's research is aimed at understanding complex combustion processes and the resulting pollutant formation. One challenging aspect of this research is to examine and describe the early combustion behavior of coal, a chemical reaction called pyrolysis. The procedure involves measuring certain features of the chemical structure of coal particles as they react and then describing this behavior with computer models. The chemical percolation devolatilization (CPD) model was developed to describe pyrolysis behavior based on measured chemical structure features of coals. This work has been applied to nitrogen-pollutant release and soot formation from coal; to pyrolysis of biomass, black liquor, and live plants (i.e., forest fires); and even to rigid closed-cell foams. Current experiments are being conducted at high pressure to support integrated gasification/combined cycle (IGCC) systems.

Another research interest is gas turbine combustion. Gas turbine combustors are highly turbulent and operated near flammability limits to prevent NO_X production. Advanced laser diagnostics (LDA, CARS, and PLIF) are used to examine details of the combustion process. Comprehensive modeling efforts include a joint scalar-velocity probability density function (PDF) approach to account for chemistry-turbulence interactions.

Finally, pure hydrocarbon compounds are being examined in a fuel-rich flat-flame reactor to study the chemical pathways of soot formation. Collected samples are analyzed with solid-state ^{13}C NMR spectroscopy and high-resolution mass spectrometry to show chemical structures of aerosol soot precursors generated from compounds such as toluene, biphenyl, and phenanthrene. This work will lead to better descriptions of the soot formation process from jet and diesel fuels.



Soot cloud formed from pyrolysis of coal particles at fuel-rich conditions in the BYU flat-flame burner facility.

PUBLICATIONS

J. Hong, W. C. Hecker, and T. H. Fletcher, "Improving the Accuracy of Predicting Effectiveness Factors for m-th Order and Langmuir Rate Equations in Spherical Coordinates," *Energy and Fuels,* **14,** 663–670 (2000).

S. Perry, T. H. Fletcher, R. J. Pugmire, M. S. Soum, "A Global Free-radical Mechanism for Light Gas Nitrogen Release from Coal during Devolatilization," *Energy and Fuels,* **14,** 1094–1102 (2000).

H. Mallampalli, T. H. Fletcher, and J.Y. Chen, "Evaluation of CH_4/NO_X Reduced Mechanisms Used for Modeling Lean Premixed Turbulent Combustion of Natural Gas," *Journal of Engineering for Gas Turbines and Power,* **120,** 703–712 (1998).

A. L. Brown and T. H. Fletcher, "Modeling Soot Derived from Pulverized Coal," *Energy and Fuels,* **12,** 745–757 (1998).

Hugh B. Hales, Professor (1996–present). ScD, Massachusetts Institute of Technology (1967). MS and BS, University of Utah (1963 and 1962). Professor of Chemical Engineering and Head of International Reservoir Simulation Research Institute, Brigham Young University (1996–present).

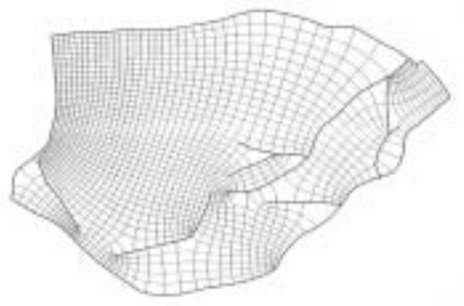
RESEARCH ACTIVITIES OF PROFESSOR HUGH B. HALES

Dr. Hugh Hales researches reservoir simulation for the petroleum industry. Reservoir simulation computerizes the flow of fluids through underground oil reservoirs composed of porous rock. Reservoir simulators allow petroleum companies' engineers to determine the production histories of their oil fields using a large number of development plans. For example, water, CO_2, nitrogen, surfactants, or steam may be injected into a reservoir to enhance its oil production. By making virtual simulations of reservoir performance, engineers can optimize the actual production, insuring that the most hydrocarbons will be produced at the least cost.

Reservoir simulation started 30 years ago and has grown steadily as computers have become more powerful. Despite the growth of computers in recent decades, however, reservoir simulation still taxes even the largest and fastest systems. The need for research on improved mathematics, which will allow faster and more accurate simulations, has never been greater. The emergence of several new technologies makes the need for such research critical.

Automatic history matching allows computers to fine-tune the voluminous data describing the reservoir by running simulations with slightly differing data to create a match between actual and simulated histories. Geostatistics provides a large number of reservoir descriptions that have probability of representing the actual reservoir. Simulation of each of these descriptions then provides the probability of various production levels throughout the life of the field.

Automatic optimization techniques use many successive simulations to systematically determine the reservoir development plan that provides the best possible reservoir recovery and income.



Curvilinear orthogonal grids provide fast and accurate simulations of reservoirs with complex geometries. They result from conformal mapping of the complex geometry into a rectangle. Hence they can be used on simulators that use Cartesian grids by simply modifying the permeability, porosity, and well data.

PUBLICATIONS

H. B. Hales, "A Method for Creating 2-D Orthogonal Grids Which Conform to Irregular Shapes," *SPE Journal 2,* **1,** 115–124 (1996).

H. B. Hales, "The Importance of Reservoir Simulation Grids Which Honor Permeability Variations," *MEPTEC Memorandum*, **LM950718-1,** July 18, 1995.

H. B. Hales, "Enhanced Curvilinear Orthogonal Reservoir Simulation Grid Generation," *MEPTEC Memorandum*, **LM950717-1,** July 17, 1995.

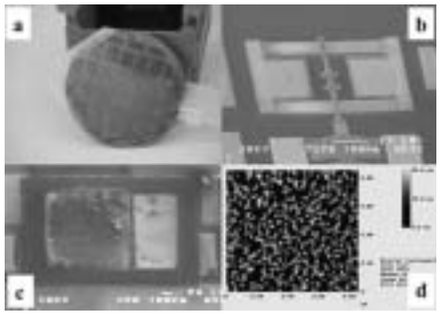
H. B. Hales, "A Method for Creating 2-D Reservoir Simulation—A Benchmark Study," *MEPTEC Memorandum*, **LM950307-2**, March 7, 1995.

John N. Harb, Professor (1988–present). PhD and MS, University of Illinois, Urbana (1988 and 1986). BS, Brigham Young University (1983).

RESEARCH ACTIVITIES OF PROFESSOR JOHN N. HARB

Professor Harb conducts research in electrochemical engineering, which includes a wide range of topics of technological importance that are governed by electrochemical phenomena. Of particular interest are energy storage devices (e.g., batteries), microfabricated electrochemical devices, and the fundamental processes that govern electrodeposition and dissolution. His work has traditionally included both modeling and experiment; molecular modeling has recently been added as an important computational research tool.

Battery development and performance represents the critical step in the development of several important future technologies including electric vehicles and hybrid-electric vehicles. Batteries are also needed for microsystems as part of a new generation of small, integrated systems. In response to this need, batteries as thin as a human hair have been made in the Integrated Microelectronics Laboratory (IML) at BYU using the same low-cost, high-volume fabrication processes used to make MEMS (MicroElectro Mechanical Systems) and integrated circuits. Working collaboratively with mechanical and electrical engineers, our department has integrated these batteries with other microsystem components developed at BYU. This work is being extended to utilize electrochemical methods for the fabrication of MEMS and other micro and nano devices. Other projects include the development of self-assembled nanopower devices in collaboration with investigators from the Departments of Chemistry and Physics at BYU. In addition, a combination of experiments and molecular modeling is being used to examine the fundamental aspects of electrodeposition in order to more effectively use this technique for micro and nanofabrication.



(a) Wafer containing >1200 microbatteries, (b) thermomechanical microactuator (with L. Howell, Mechanical Engineering), (c) SEM micrograph of Ni/Zn microbattery, (d) AFM image of proteins for use in nanoelectrochemical systems (with R. Davis, Physics, and G. Watt, Chemistry).

PUBLICATIONS

J. N. Harb, R. M. LaFollette, R. H. Selfridge, and L. L. Howell, "Microbatteries for Self-sustained Hybrid Micropower Supplies," *Journal of Power Sources*, **104,** 46 (2002).

C. D. Lott, T. W. McLain, J. N. Harb, and L. L. Howell, "Modeling the Thermal Behavior of a Surface Micromachined Linear-displacement Thermomechanical Microactuator," *Sensors and Actuators, A Physical*, **101,** 239–250 (2002).

P. H. Humble, J. N. Harb, and R. M. LaFollette, "Microscopic Nickel-zinc Batteries for use in Autonomous Microsystems," *Journal of Electrochemical Society,* **148,** A1357–A1361 (2001).

J. N. Harb and R. M. LaFollette, "Mathematical Model of the Discharge Behavior of a Spirally Wound Lead-acid Cell," *Journal of Electrochemical Society,* **146,** 809–818 (1999).

J. N. Harb, V. H. Johnson, and D. Rausen, "Use of a Fundamentally based Lead-acid battery Model in Hybrid Vehicle Simulations," *Tutorials in Electrochemical Engineering—Mathematical Modeling,* **99,** 14 (1999).

William C. Hecker, Associate Professor (1982–present). PhD, University of California, Berkeley (1982). MS and BS, Brigham Young University (1975 and 1974). AIChE Student Chapter Advisor (1984–1997, 2001–present).

RESEARCH ACTIVITIES OF PROFESSOR WILLIAM C. HECKER

Dr. Hecker's specialities are chemical kinetics and heterogeneous catalysis, with specific interests in NO_x reduction catalysis, char combustion kinetics, and FTIR spectroscopy of adsorbed species. He seeks to gain fundamental kinetic/mechanistic information about chemically reactive catalytic and non-catalytic systems by measuring reaction rates and surface properties. This information is then used to develop predictive models.

For 20 years Dr. Hecker has studied the catalytic reduction of NO_x over a variety of catalysts (including oxide and zeolite-supported rhodium, rhodium-bimetallics, copper, etc.) using different reducing agents (CO, H_2, CH_4, char). Infrared spectroscopy is used to study reactions *in situ* and gain information regarding catalyst surfaces and adsorbates. Dr. Hecker has developed a quantitative technique that uses CO as an infrared surface probe (CISP) to determine the active surface area and surface properties of solid catalysts. He has also completed an extensive study on the reduction of NO_x by coal char, studying the effects of burnout, catalytic mineral matter, and flue gases.

Dr. Hecker's group has developed a char oxidation model (BCOM) that predicts high-temperature char oxidation behavior over a wide range of conditions and char types. Group members do kinetic measurements of char oxidation at both high and low temperatures using a drop tube reactor, flat-flame burner, and TGA. They have shown that CaO inherent in the mineral matter of coal char acts as a catalyst in both char oxidation and NO_x reduction. The group is currently studying the kinetics of char oxidation at high pressure.

Dr. Hecker working with a student on the FTIR flow reactor apparatus.

PUBLICATIONS

W. C. Hecker, P. M. Madsen, M. R. Sherman, J. W. Allen, R. J. Sawaya, and T. H. Fletcher, "High Pressure Intrinsic Oxidation Kinetics of Two Coal Chars," *Energy and Fuels (*March/April 2003).

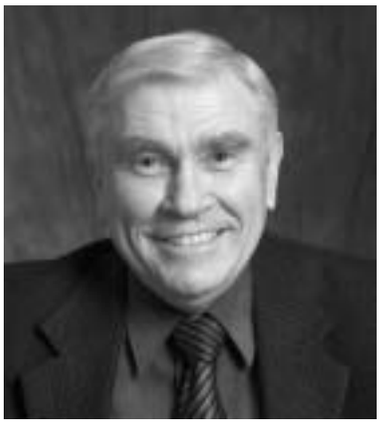
R. E. Terry, J. N. Harb, W. C. Hecker, and W. V. Wilding, "Definition of Student Competencies and Development of an Educational Plan to Assess Student Mastery Level," *International Journal of Engineering Education* **18,** no. 2, 225–235 (2002).

F. Guo and W. C. Hecker, "Kinetics of NO Reduction by Char: Effects of Coal Rank," *Twenty-Seventh Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, 3085–3092 (1998).

W. C. Reade, K. W. Morris, and W. C. Hecker, "Modeling the Effects of Burnout on High-temperature Char Oxidation," *Coal Science,* J. A. Pajares and J. M. D. Tascon (eds.), Elsevier Science B.V., Amsterdam, **24,** 639–642 (1995).

C. H. Bartholomew and W. C. Hecker, "Catalytic-reactor Design: Keep the Catalyst in Mind from the Beginning," invited feature report in *Chemical Engineering Magazine*, 70–75 (1994).

P. B. Rasband and W. C. Hecker, "Catalyst Characterization Using Quantitative FTIR: CO on Supported Rh," *J. Catalysis*, **139,** 551–560 (1993).



John L. Oscarson, Professor (1974–present). PhD and MES, University of Michigan (1985 and 1972). BS, Brigham Young University (1968). Codirector of DIPPR Thermophysical Properties Laboratory (1997–present).

RESEARCH ACTIVITIES OF PROFESSOR JOHN L. OSCARSON

Dr. Oscarson works in the general area of thermodynamics. One area where he is actively doing research is the investigation of the thermodynamics of aqueous inorganic solutions at high temperatures (up to 400°C) and pressures (up to 25 MPa). He uses a high-temperature, high-pressure, isothermal-flow calorimeter to measure the heats involved when aqueous solutions are mixed under these extreme conditions. Interpreting the heat data at temperatures below about 350°C allows him to model activity coefficients, heats of reaction, and equilibrium constants at these temperatures. He is presently working on a new thermodynamic model that correlates the data at temperatures above 350°C, where the density of the solutions is highly dependent on the pressure. These models are needed in reducing boiler tube corrosion in power-generating plants and in the emerging technology of oxidizing waste in aqueous solutions at temperatures and pressures above the critical point of water. Dr. Oscarson is also investigating the reaction heats of simple biomolecules as a function of temperature (0 to 125°C). The change of the ΔH of reaction with temperature, ΔC_p, is an indicator of the types of reactions occurring and if the molecules are stable at a given temperature. He is also one of the principle investigators involved in maintaining the DIPPR 801 database, which includes correlating and evaluating the thermophysical properties of pure components.

High-temperature (up to 420°C) flow calorimeter used to measure heats of dilution and reaction in aqueous solutions.

PUBLICATIONS

S. Fuangswasdi, J. L. Oscarson, and R. M. Izatt, "A New Flow Calorimeter Using a Eutectic Molten Salt as the Temperature Control Medium," *Thermochimica Acta,* **373,** 13–22 (2001).

J. L. Oscarson, B. A. Palmer, S. Fuangswasdi, and R. M. Izatt, "A New Model Incorporating Ion Dissociation for Sodium Chloride Solutions near the Critical Point of Water," *Ind. Eng. Chem. Res.,* **40,** 2176–2182 (2001).

J. L. Oscarson, H. K. Grimsrud, and S. E. Gillespie, "Heats of Mixing of Gaseous CO_2/CH_4 Mixtures with Aqueous Solutions of Methyldiethanolamine and Diethanolamine," *Thermochimica Acta*, **351,** 9–20 (2000).

X. X. Zhang, J. L. Oscarson, R. M. Izatt, P.C. Schuck, and D. Li, "Thermodynamics of Macroscopic and Microscopic Proton Ionization from Protonated 4-aminobenzoic Acid in Aqueous Solution from 298.15 to 393.15 K," *J. Phys. Chem. B.*, **104,** 8598–8605 (2000).

William G. Pitt, Professor (1987–present). PhD, University of Wisconsin, Madison (1987). BS, Brigham Young University (1983).

RESEARCH ACTIVITIES OF PROFESSOR WILLIAM G. PITT

Dr. Pitt's research group was the first to discover that the killing effect of many antibiotics is enhanced by the application of ultrasound. They have found that enhanced killing increases with power density, decreases with increasing frequency, and is enabled by both continuous and pulsed waveforms. In nearly all cases in which a bacterial biofilm has formed on a medical implant, the infection can never be cured, even by aggressive antibiotic therapy, and thus the implant must be removed and replaced. Dr. Pitt hopes to apply this technology to eliminate bacterial infections on implants without resorting to surgical procedures.

His research has shown that anticancer drugs can be sequestered inside small micelles that can be injected into the bloodstream and then travel throughout the body. Dr. Pitt's goal is to make a drug carrier that will release the drug in the body only when activated by ultrasound. The advantages to cancer therapy are obvious.

The research group employs tissue engineering to grow cells on solid substrates. Usually these cells don't grow well because they "recognize" the foreign surface. The group is working on a technology to mislead the cells by covalently attaching hyaluronic acid to the metal or polymeric surface. It has submitted one patent for attaching hyaluronic acid to polymers and is working to attach them to orthopedic metals such as stainless steel and titanium alloys.

Dr. Pitt developing polymeric drug delivery systems for chemotherapy.

PUBLICATIONS

J. L. Nelson, B. L. Roeder, J. C. Carmen, R. Roloff, and W. G. Pitt, "Ultrasonically Activated Chemotherapeutic Drug Delivery in a Rat Model," *Cancer Research*, **62** (24), 7280–7283 (2002).

A. M. Rediske, B. L. Roeder, J. L. Nelson, R. L. Robinson, G. B. Schaalje, R. A. Robinson, and W. G. Pitt, "Pulsed Ultrasound Enhances the Killing of *Escherichia Coli* Biofilms by Aminoglycoside Antibiotics in Vivo," *Antimicrobial Agents and Chemotherapy,* **44,** 771–772 (2000).

G. A. Husseini, R. I. El-Fayoumi, K. L. O'Neill, N.Y. Rapoport, and W. G. Pitt, "DNA Damage Induced by Micellar-delivered Doxorubicin and Ultrasound: Comet Assay Study," *Cancer Letters,* **154,** 211–216 (2000).

J. Pruitt, G. Husseini, N.Y. Rapoport, and W. G. Pitt, "Stabilization of Pluronic P-105 Micelles with an Interpenetrating Network of N, N-d iethylacrylamide," *Macromolecules*, **33,** 9306–9309 (2000).

Richard L. Rowley, Professor (1984–present). PhD, Michigan State University (1978). BS, Brigham Young University (1974). Codirector of DIPPR Thermophysical Properties Laboratory (1997–present).

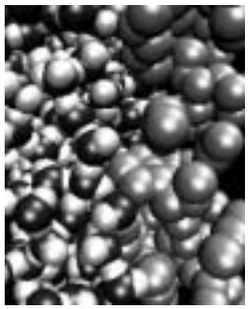
RESEARCH ACTIVITIES OF PROFESSOR RICHARD L. ROWLEY

Dr. Rowley's research focuses on a combination of accurate experimental data supplemented with advanced, accurate prediction through three approaches: (1) the DIPPR database (please see the section of the brochure on DIPPR), (2) advanced computational chemistry and molecular simulations, and (3) new property prediction methods.

Current DIPPR research areas include (1) comprehensive evaluation of properties for families of compounds and (2) development of new property prediction methods.

Molecular simulations are used to understand the molecular underpinnings of thermophysical properties and to predict property values from molecular interactions. Dr. Rowley's group uses these kinds of simulations to predict the viscosity of potential new synthetic lubricants based on their molecular structure and intermolecular interactions. His group also performs simulations on systems near membranes to obtain fluid structure and transport rates in membrane pores. A current project involves simulating the electrodeposition process used in developing circuits on semiconductor chips to see how the deposition is affected by additives in the solution. Another project involves using quantum-mechanical *ab initio* calculations to improve intermolecular potential models used in simulations.

Related to the above area is the extension of these computational chemistry techniques to predict properties. One such method, quantitative structure-property relationships (QSPR), is being used to correlate structure to macroscopic properties. Using computational chemistry tools, molecular descriptors that characterize the geometry, structure, and electronic configuration of the molecules are developed. These descriptors are then correlated with macroscopic properties.



A snapshot of a molecular dynamics simulation of the liquid interface between water molecules (left) and n-hexane molecules (right).

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D. Ericksen, W. V. Wilding, J. L. Oscarson, and R. L. Rowley, "Use of the DIPPR Database for Development of QSPR Correlations: Normal Boiling Point," *Journal of Chemical Engineering Data,* **47**, 1293–1302 (2002).

P. S. Crozier and R. L. Rowley, "Activity Coefficient Prediction by Osmotic Molecular Dynamics," *Fluid Phase Equilibria,* **193,** 53–73 (2002).

J. P. Jalkanen, R. Mahlanen, T. A. Pakkanen, and R. L. Rowley, "Ab Initio Potential Energy Surfaces of the Propane Dimmer," *Journal of Chemical Physics,* **116,** 1303–1312 (2002).

P. S. Crozier, R. L. Rowley, E. Spohr, and D. Henderson, "Comparison of Charged Sheets and Corrected 3-D Ewald Calculations of Long-ranged Forces in Slab Geometry Electrolyte Systems with Solvent Molecules," *Journal of Chemical Physics*, **112,** 9253–9257 (2000).

Y. Yang, T. Pakkanen, and R. L. Rowley, "Nonequilibrium Molecular Dynamics Simulations of Shear Viscosity: Isoamyl, Alcohol, n-Butyl Acetate, and Their Mixtures," *International Journal of Thermophysics,* **21,** 703–717 (2000).

D. R. Wheeler and R. L. Rowley, "Shear Viscosity of Polar Liquid Mixtures Via Non-equilibrium Molecular Dynamics: Water, Methanol, and Acetone," *Molecular Physics,* **94,** 555–564 (1998).

Kenneth A. Solen, Professor (1976–present). PhD and MS, University of Wisconsin, Madison (1974 and 1972). BS, University of California, Berkeley (1968).

RESEARCH ACTIVITIES OF PROFESSOR KENNETH A. SOLEN

Professor Solen's research interests are in biomedical engineering, with recent emphasis on improving the compatibility of biomaterials with blood and on selectively removing blood components for therapeutic purposes.

Blood-biomaterial incompatibility includes (1) the formation of platelet aggregates (thrombi) on biomaterial surfaces, which can inhibit artificial organ function, and (2) the release of portions of the thrombi into the bloodstream (microemboli), which can block blood capillaries and damage organ systems. Dr. Solen's group studies these phenomena and the effects of hemodynamics and drugs on their development. One discovery is that clinical hypothermia (routinely used during cardiopulmonary bypass) causes the blood platelets of some patients to form aggregates (microemboli) with strength to block microvascular flow and possibly contribute to the neurologic dysfunction associated with open-heart surgery.

The selective removal of blood components during clinical procedures may have potential benefits. For example, an anticoagulant is routinely infused into patients undergoing cardiopulmonary bypass, but some patients react to the anticoagulant. Dr. Solen's group is exploring the removal of some clotting factors from the patient's blood as a strategy to reduce the need for anticoagulant infusion. Additionally, fibrin sealants are useful in reducing uncontrolled bleeding following surgery, but the use of donor blood in the preparation of the fibrin poses a risk of transmitting blood-borne pathogens. Dr. Solen's group is developing a technique to collect fibrinogen (a precursor to fibrin) from small volumes of the patient's own blood as a safe method of preparing the tissue sealant.

Computer rendering of a hemodialysis catheter in preparation for modeling blood-material interactions on the catheter surface.

PUBLICATIONS

K. A. Solen, S. Sukavaneshvar, Y. Zheng, B. Hanrahan, M. W. Hall, P. Goodman, B. Goodman, S. F. Mohammad, "A Light-scattering Instrument to Detect Thromboemboli in Blood," *J. Biomed. Optics*, **8,** 70–79 (2003).

M. W. Hall and K. A. Solen, "Hypothermia-induced Platelet Aggregation in Human Blood in an In-vitro Model: The Dominant Role of Blood-material Interactions," *J. Biomed. Mater. Res.*, **59,** 528–534 (2002).

M. W. Hall, P. D. Goodman, S. M. Alston, and K. A. Solen, "Hypothermia-induced Platelet Aggregation in Human Blood in an In-vitro Model: Identification of a High Responder Subpopulation," *Am. J. Hematol.*, **69,** 45–55 (2002).

S. Sukavaneshvar, K. A. Solen, and S. F. Mohammad, "An In-vitro Model to Study Device-induced Thrombosis and Embolism: Evaluation of the Efficacy of Tirofiban, Aspirin, and Dipyridamole," *Thromb. Haem,* **83,** 322–326 (2000).

S. Sukavaneshvar, G. M. Rosa, K. A. Solen, "Thrombosis and Embolism in a Stenosis-Stent Model: Contribution of Hemodynamics," *Ann. Biomed. Engr.*, **28** (2), 182–193 (2000).

P. Goodman, M. W. Hall, S. Sukavaneshvar, K. A. Solen, "An In-vitro Model for Studying the Effects of Hemodynamics on Device-induced Thromboembolism in Human Blood," *ASAIO J.,* **46,** 576–578 (2000).

Ronald E. Terry, Professor (1987–present). PhD, Brigham Young University (1976) BS, Oregon State University (1971).

RESEARCH ACTIVITIES OF PROFESSOR RONALD E. TERRY

Heavily involved in engineering education, Professor Terry led an effort at BYU to inform college faculty about student learning styles. To this end he has coauthored a monograph on the application of the Kolb Learning Style Theory entitled *Teaching Through the Cycle: Application of Learning Style Theory to Engineering Education at Brigham Young University.* Numerous engineering colleges have used the monograph to educate their faculty regarding student learning styles and teach them how to design activities to reach all types of learners. Other topics that Dr. Terry has actively researched include cooperative learning, assessment practices, and faculty development issues.

Reservoir engineering and developing technology for underdeveloped areas of the world are the major areas of Dr. Terry's technical interest. To help engineers apply scientific principles to determine the most efficient method of producing natural gas and crude oil from underground reservoirs, Professor Terry has coauthored a popular textbook called *Applied Petroleum Reservoir Engineering.* And, working on his other interest, he and a colleague have recently been pursuing a water analysis project in Bolivia as a precursor for possible future work.

Dr. Terry applying some of his research relative to student learning styles.

PUBLICATIONS

R. E. Terry and K. Sandholtz, "A New Look at Faculty Development: Building a Satisfying, Valued Career in Academia," *Professional and Organizational Development Annual Meeting,* Lake Harmony, Pennsylvania (14–16 October 1999).

W. V. Wilding, J. N. Harb, R. E. Terry, and W. C. Hecker, "Maximizing the Benefits of Developing an Educational Plan to Meet the ABET 2000 Criteria," *Proceedings of 1999 ASEE Annual Conference,* Charlotte, North Carolina (20–23 June 1999).

R. E. Terry and K. Sandholtz, "Empowering Graduates to Manage Professional Careers for Greater Satisfaction and Contribution," *Proceedings of 1999 ASEE Annual Conference,* Charlotte, North Carolina (20–23 June 1999).

J. N. Harb, R. E. Terry, P. K. Hurt, and K. J. Williamson, *Teaching Through the Cycle: Application of Learning Style Theory to Engineering Education at Brigham Young University,* 2nd Edition, Provo, UT, BYU Press (1995).

B. C. Craft, and M. Hawkins, revised by R. E. Terry, *Applied Petroleum Reservoir Engineering,* Englewood Cliffs, NJ: Prentice Hall (1991).

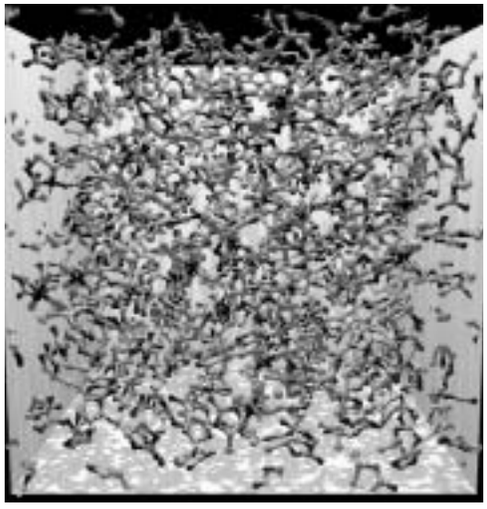
Dean R. Wheeler, Assistant Professor (2003–present). PhD, University of California, Berkeley (2002). BS, Brigham Young University (1996).

RESEARCH ACTIVITIES OF PROFESSOR DEAN R. WHEELER

Dr. Wheeler and his newly formed research group are working to better understand and improve performance of electrochemical systems and processes. The group is part of a worldwide effort to improve lithium batteries so they can be used economically in electric vehicles. In collaboration with Professors Harb and Rowley, the Wheeler group seeks to improve understanding of the electrochemical deposition and dissolution processes used in semiconductor device fabrication in order to help adapt these processes to smaller length scales.

The group's primary research method is to perform molecular-scale computer simulations (such as molecular dynamics) to elucidate the connections between microscopic and macroscopic behavior—that is, how the interactions of molecules influence thermodynamic and transport properties of materials. The molecular simulations serve as a means of estimating properties when experimental data is difficult to obtain. Additional methods used by the group include continuum-scale computer models of electrochemical systems, as well as experiments to determine thermodynamic and transport properties. Dr. Wheeler and his students collaborate with other groups in order to learn and to teach new modeling and experimental techniques.

Current and planned research includes simulations and experiments for understanding multicomponent transport in lithium batteries and modeling and experiments for understanding the deposition of copper interconnects on silicon wafers.



Configuration snapshot from a molecular simulation of 1 molar LiPF6 in propylene carbonate, an electrolyte used in lithium batteries.

PUBLICATIONS

J. Newman, K. E. Thomas, H. Hafezi, and D. R. Wheeler, "Modeling of Lithium-ion Batteries," *Journal of Power Sources,* in press (2003).

D. R. Wheeler and J. Newman, "A Less Expensive Ewald Lattice Sum," *Chemical and Physical Letters*, **366,** 537–543 (2002).

D. R. Wheeler and R. L. Rowley, "Shear Viscosity of Polar Liquid Mixtures via Non-equilibrium Molecular Dynamics: Water, Methanol, and Acetone," *Molecular Physics*, **94,** 555–564 (1998).

W. Vincent Wilding, Professor (1994–present). PhD, Rice University (1985). BS, Brigham Young University (1981). Codirector of DIPPR Thermophysical Properties Laboratory (1997–present).

RESEARCH ACTIVITIES OF PROFESSOR W. VINCENT WILDING

Design and development of chemical processes are strongly dependent upon accurate thermophysical property values. Dr. Wilding obtains these values through careful experimental work and from reliable prediction techniques.

Pure-component properties are the focus of the BYU-DIPPR Thermophysical Properties Laboratory, which is home to DIPPR Project 801: Evaluated Process Design Data (please see the section of the brochure on DIPPR). Literature surveys, evaluation of experimental data, evaluation of prediction techniques, development of new prediction techniques, and experimental measurement of essential properties are all included in the project's activities.

Experimental measurements of thermophysical properties complement the database work. Accurate measurements of vapor pressures, densities, surface tension, viscosity, and thermal conductivity are made in our laboratory. Mixture data are also essential to process design, and accurate phase equilibrium measurements are performed to provide activity-coefficient information. Experimental measurements support the development of new correlations and help to test property prediction techniques.

Studies to understand and mitigate contaminant transport in the subsurface constitute a growing area of research. Thermodynamics equilibrium dictates the partitioning of contaminants between vapor, liquid, aqueous, and adsorbed phases. Understanding the forces that affect transport help to remediate contaminated sites and contribute to the design of control strategies.

Educational plans to improve student learning and to maximize the benefits of outcomes-based education are the focus of collaborative studies with several other members of the chemical engineering faculty. These studies provide impetus and techniques to continually improve the education of chemical engineering students.

Dr. Wilding helping students with thermophysical property measurements.

PUBLICATIONS

W.V. Wilding, K. L. Adams, A. E. Carmichael, J. B. Hull, T. C. Jarman, and T. L. Marshall, "Vapor-Liquid Equilibrium Measurements on Three Binary Mixtures: Allyl Alcohol / Acetonitrile, 2-Butoxyethanol / Acetic Acid, 1-Methoxy-2-Propanol / 2,3-Epoxy-1-Propanol," *Journal of Chemical and Engineering Data*, **47** (4), 740–747 (2002).

R. E. Terry, J. N. Harb, W. C. Hecker, and W.V. Wilding, "Definition of Student Competencies and Development of an Educational Plan to Assess Student Mastery Level," *International Journal of Engineering Education,* **18** (2), 225–235 (2002).

R. L. Rowley, J. L. Oscarson, and W.V. Wilding, "DIPPR® Project 801: Evaluated Process Design Data," *Fluid Phase Equilibria,* 150–151 (1998).

H. L. Wilson and W.V. Wilding, "Pressure-Volume-Temperature Behavior of Binary Mixtures of Hydrogen Fluoride with HCFC-22, HFC-32, and HFC-134a," *Fluid Phase Equilibria,* 150–151 (1998).

PROGRAM

Numbers

Faculty: 14 (13 PhD and 1 ScD)
Graduate students: 38

Graduate Program Courses

Computer applications in chemical engineering, transport phenomena, thermodynamics, simulation, kinetics/catalysis, combustion, semiconductors, materials, and biomedical.

Starting Salaries

Salaries offered to our graduates are at or above national averages.

FINANCIAL AID

All of our current students receive some form of support in the form of tuition, stipends, teaching assistantships, or fellowships.

Teaching Assistantships

Money is available to pay up to 20 hours per week teaching. MS candidates are required to work as a teaching assistant 10 hours sometime during their residency. PhD candidates are required to work as a teaching assistant 20 hours sometime during their residency.

Research Assistantships

Most professors have funding to support graduate students.

Fellowships

Many of our students have received National Science Foundation fellowships and other national and international fellowships. We invite all qualified applicants to apply for such fellowships.

DEPARTMENT HISTORY

The teaching of chemical engineering at Brigham Young University was officially initiated in 1955 with the renaming of the Department of Chemistry to the Department of Chemistry and Chemical Engineering. Only one full-time faculty member taught the chemical engineering courses at that time. In 1958 a separate Department of Chemical Engineering was formed, this time with three faculty members. The undergraduate program was first accredited in 1961 and has remained so ever since. A master's degree in chemical engineering was approved in 1962, and the PhD program received approval in 1968. From these beginnings the department has grown to its present size of 14 full-time faculty, around 350 undergraduate students, and approximately 45 graduate students.

BRIGHAM YOUNG UNIVERSITY Founded in 1875, Brigham Young University is sponsored by The Church of Jesus Christ of Latter-day Saints and is part of the Church Educational System (CES), which serves approximately 1,200,000 people worldwide. Nearly 30,000 students from more than 100 countries are enrolled at BYU's Provo, Utah, campus. Almost half of them have lived outside the U.S., and three-fourths are fluent in at least two languages.

The variety of cultures and backgrounds, coupled with an institutional commitment to the gospel of Jesus Christ, adds to an academic experience that challenges the mind while feeding the spirit—whether you belong to the Church or to one of the 20 other denominations represented on campus.

DEPARTMENT OF CHEMICAL ENGINEERING