A program on . . .

ADVANCED COMBUSTION ENGINEERING

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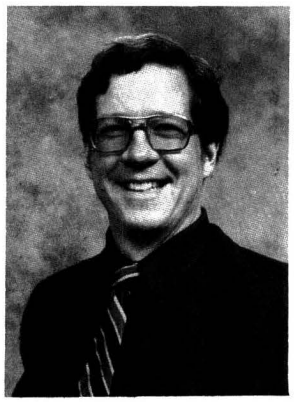
OUR NATION'S BASIC and high technology industries are highly dependent on an adequate supply of energy, the production of which depends upon combustion technology. The future survival of these industries will hinge on the ability to utilize more efficiently, through advanced combustion technology, our nation's readily available, low-cost fuel resources.

There are unfortunately several formidable roadblocks threatening the realization of these critically needed developments: (1) commitment of combustion-based industries to out-dated technologies, (2) environmental and operational problems in the utilization of low-cost, low-grade fuels, (3) insufficient understanding of combustion fundamentals, and (4) lack of communication, collaboration and cooperation among investigators in academic, industrial and governmental research and development communities.



Calvin H. Bartholomew received his BS degree from Brigham Young University and his MS and PhD degrees in chemical engineering from Stanford University. He spent a year at Corning Glass Works and a summer at Union Oil as a visiting consultant before joining the chemical engineering department at Brigham Young University in 1973. He is presently professor, head of the BYU Catalysis Laboratory, and Associate Director of the Advanced Combustion Engineering Research Center. Recipient of the Karl G. Maeser Research Award, he has authored over 70 scientific papers and 5 major reviews in the fields of heterogeneous catalysis and catalyst deactivation. His major research and teaching interests are heterogeneous catalysis, char combustion, kinetics and reactor design, Moessbauer spectroscopy, surface science, and air pollution control.

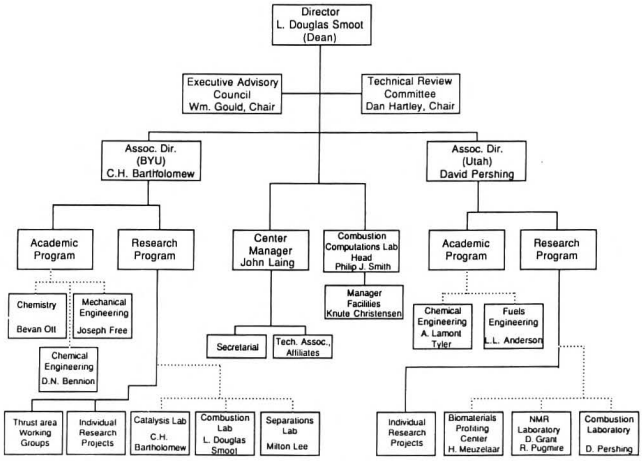


FIGURE 1. Management structure of the Advanced Combustion Engineering Research Center

To address the removal of these roadblocks, the Advanced Combustion Engineering Research Center (ACERC) was established in the summer and fall of 1985 as a cooperative effort among Brigham Young University (BYU), the University of Utah (U of U), two national laboratories (Sandia National Labs and Los Alamos National Labs), and 23 industrial/research organizations located throughout the United States. The departments of chemical engineering (BYU and U of U), chemistry (BYU and U of U), fuels engineering (U of U), and mechanical engineering (BYU) were involved in the formation of this new center. Headquarters were established at BYU. The organization of the new center, consisting of a Directorate, an Executive Advisory Council and Technical Review Committee, is illustrated in Figure 1. Members of the management team consisting of the directorate and coordinators for research, education, and information dissemination are listed in Table 1, while members of the Executive Advisory Council are listed in Table 2. Listed in Table 3 are companies and

laboratories which have subscribed as technical partners of the center.

In the fall of 1985, proposals were submitted to the National Science Foundation (NSF) and the State of Utah for funding. On May 1, 1986, BYU and the U of U were jointly awarded a $9.7 million 5-year grant from NSF as part of its Engineering Research Centers Program. This award was one of five selected from 102 proposals submitted by 74 institutions in fall 1985. Also receiving grant awards from NSF in the 1985-86 round were Carnegie-Mellon University, University of Illinois-Urbana, Lehigh University and Ohio State University.

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In addition to the funds from NSF, the center will receive approximately $3.5 million from the two universities, $500,000 from the State of Utah, and over $500,000 from private industry, for a total of about $14 million for the five years. During the first year the total ACERC budget was $3.2 million.

RESEARCH OBJECTIVES AND PROGRAM

Objectives. Since combustion is a very broad field, a focus is essential in order to make a significant contribution. ACERC's research program has been designed to address the most significant research priorities for U. S. competitiveness in combustion technology while removing the roadblocks mentioned above. *The principal objective of ACERC is to develop and implement, within 5 years, advanced computer-*

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TABLE 1
ACERC Management

Director
L. Douglas Smoot
Dean of Engineering and Technology
Head of the Combustion Laboratory

Associate Directors and Research Coordinators

BYU	U of U
Calvin H. Bartholomew	David W. Pershing
Professor of Chem. Eng.	Professor of Chem. Eng.
Head of the Catalysis Lab	Assoc. Dean of Grad. School

Academic Coordinator

Calvin H. Bartholomew	David M. Bodily
Professor of Chem. Eng.	Professor of Fuels Eng.
	Assoc. Dean of Mines & Min.

External Relations Coordinator

John C. Laing	Ronald J. Pugmire
Manager, ACERC	Prof. of Fuels Eng.
	Assoc. Vice Pres. of Res.

TABLE 2
Executive Advisory Council

- **William Gould,** Chairman, Retired Chief Executive Officer of Southern California Edison and EPRI Chairman
- **Christian Bolta,** Director of Technology Strategy, Combustion Engineering, Inc.
- **Dan Hartley,** Vice President of Sandia National Laboratories
- **George Hill,** Professor of Chemical Engineering at the University of Utah and former Director of the office of Coal Research and EPRI
- **Eric Reichl,** Consultant and Retired President of the Conoco Coal Development Company
- **Adel Sarofim,** Professor of Chemical Engineering, MIT
- **George Watkins,** Executive Director of the Empire State Electric Energy Research Corporation

TABLE 3
Technical Partners of ACERC

TECHNICAL ASSOCIATES

- **Advanced Fuel Research, Inc.**
- **Babcock and Wilcox**
- **Combustion Engineering, Inc.**
- **Consolidated Coal Co.**
- **Convex Computer Corp.**
- **Electric Power Research Institute**
- **Empire State Electric Energy Research Corp.**
- **Foster-Wheeler Development Corp./IHI (Japan)**
- **Gas Research Institute**
- **Morgantown Energy Tech. Center**
- **Pittsburgh Energy Tech. Center**
- **Tennessee Valley Authority**
- **Utah Power and Light Co.**

TECHNICAL AFFILIATES

- **General Motors Corp. (Alison Gas Turbine Div.)**
- **Chevron Research Co.**
- **Corning Glass Works**
- **Dow Chemical USA**
- **General Electric Co.**
- **Los Alamos National Laboratory**
- **Pyropower Corp.**
- **Questar Development Corp.**
- **Shell Development Co.**
- **Southern California Edison**

COMBUSTION ENGINEERING

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aided design methods in U. S. industry, with emphasis on clean and efficient use of low-grade fuels. The approach is to integrate kinetic and mechanistic data, physical/chemical fuel property data, and process performance characteristics into comprehensive state-of-the-art computer models to be used in the simulation, design and optimization of advanced combustion processes. The underlying philosophy is that a fundamental systems approach applied to carefully selected systems will have wide application to many important combustion problems. The products of the new center will include: (1) new computer-aided-design combustion technology, (2) new understanding of combustion mechanisms and their relation to fuel properties, (3) improved process strategies, and (4) students educated in the fundamentals of combustion engineering who can solve a wide range of problems.

Program. Research projects are focused in six fundamental areas: (1) fuels characterization and reaction mechanisms, (2) fuel minerals, fouling and slagging, (3) pollutant formation and control, (4) comprehensive model development, (5) process characteristics/model evaluation, and (6) exploratory areas. The first five areas are the key elements needed for complete design, optimization and control of advanced technology for combustion processes. The following three research subjects, specifically identified by a blue ribbon panel as among the potentially most productive for the near-term, are receiving particular emphasis: (1) comprehensive and generalized modeling of coal combustion processes, (2) identification of the relationships between chemical/physical properties of fuels at the molecular level and reaction processes, and (3) fundamentals of formation and control of sulfur and nitrogen emissions. Exploratory research presently includes hazardous waste disposal and may expand in the future to fluidized beds, catalytic combustion, or catalytic reduction of NO_x. The heart of the center's research program presently consists of about thirteen research projects at BYU and U of U, funded on the basis of excellence and pertinence to the focus/subject areas, as well as eight research projects funded by a consortium of companies through the center. Some of the key investigators involved in some of these projects are listed in Table 4.

INDUSTRIAL RELATIONS AND TECHNOLOGY TRANSFER

The Executive Advisory Council (Table 2), consisting of highly placed executives and professionals, provides essential direction on the focus of the center's research and academic programs. Besides financial support, the Technical Associates of the center (Table 3) participate through representation in the Technical Review Committee and through attendance at the ACERC Annual Review. Visits and interchanges of students and faculty with industrial professionals of these companies and laboratories are also planned. Center funds will provide half-support for a visiting industrial research fellow on a continuing basis. To promote technology transfer, an annual review and a biannual technical conference are held on campus with presentations on advanced combustion from academia, government and industry. The center also disseminates new information through annual technical reports, journal publications, presentations at meetings, technical workshops, and computer networking.

ACADEMIC PROGRAM

The objective is to educate students in engineering and scientific fundamentals using the systems approach in a way that will prepare them to solve a wide range of problems. Fellowship support is provided for 4-5 graduate and 8-10 undergraduate students. A combination of 3-4 new and 20 currently available courses among six departments in four colleges at the two universities provide a broad basis for both general and specific education in combustion-related science and engineering. At the undergraduate level, students re-

TABLE 4
Key Investigators: ACERC

INVESTIGATOR	AREA OF EXPERTISE
Calvin H. Bartholomew, ChE, BYU William C. Hecker, Chem. Eng., BYU	Catalysis, Surface properties of coal and chars
David M. Grant, Chemistry, U of U Ronald J. Pugmire, Fuels Eng., U of U	NMR characterization of fuels
George Hill, Chem. Eng., U of U Henk Meuzelaar, Biomaterials Profiling Center, U of U	Coal characterization and properties correlation
Milton R. Lee, Chemistry, BYU	Chromatographic analysis of fuels
Angus Blackham, Chemistry, BYU John W. Cannon, Mech. Eng, BYU	Fouling, slagging, minerals, chemical analysis
David W. Pershing, Chem. Eng., U of U	Pollutant formation and submodels
Philip J. Smith, Chem. Eng., BYU L. Douglas Smoot, Chem. Eng. BYU	Comprehensive model development
Mike Stephensen, Civil Eng., BYU	Graphics code development
Paul O. Hedman, Chem. Eng., BYU Geoffery Germane, Mech. Eng., BYU	Process characteristics and diagnostics

ceive general exposure to systems, energy, and environmental engineering in the form of senior electives; a new undergraduate program option will be established in chemical engineering at BYU. Graduate students receive a more specific education in such topics as combustion science and engineering, kinetics, physical and chemical structure of solids and fuels, and process modeling and control. Selected courses, seminars, and ad hoc seminars from visiting industrial lecturers at both universities are offered to students in a coordinated curriculum. Efforts are being made to optimize the use of remote circuit TV and a shuttle-bus system between the two campuses. Graduate and undergraduate participation in combustion research is also stimulated by research fellowships and assistantships. A continuing education program is being organized to serve the needs of industrial engineers and scientists for professional development in combustion related subjects and to train them in the use of simulation codes using state-of-the-art computer graphics workstations in our new Computations Center.

MAJOR ACCOMPLISHMENTS OF THE FIRST YEAR

During the first year of its existence, the center initiated and funded thirteen new projects, purchased a new Convex Mini Supercomputer, and completed construction of a new computations laboratory that features state-of-the-art work stations for computer code development and demonstration. A proposal for a link to the NSF-supported San Diego Cray for running these codes was submitted to NSF and accepted. Workshops on comprehensive modeling, fouling and slagging, and other advanced combustion topics were conducted; organizational meetings for ACERC faculty, the Executive Advisory Council, and the Technical Review Committee were held; working groups involving prominent scientists and engineers in each of the thrust areas were organized; visits were made to other cooperating laboratories, including Sandia National Laboratories, for purposes of establishing collaboration; and a number of prominent engineers and scientists were invited to lecture in the center.

Significant progress was made on twenty-one research projects in the six thrust areas of research presently emphasized in the center. These projects included eight active research projects funded by the foundational consortium grant. A summary of the accomplishments of the ACERC and consortium projects can be obtained from the author. Consortium projects were active for the entire fiscal year, while ACERC projects were generally initiated in September, 1986, and progress thus covers only an eight month period. Even so, several important accomplishments are noted. Of particular significance was the development and demonstration of a 3-D combustion code for non-reacting, gaseous flows. Work on a significantly improved radiation submodel was successfully completed, while submodel elements for SO_x-sorbent capture, fouling-slagging and carbon nonequilibrium were identified. Further evaluation was completed on an NO_x submodel and a comprehensive 2-D combustion code (PCGC-2) previously developed in the combustion laboratory. A new algorithm for graphical representation of combustion model predictions was developed. Standard ACERC coals were identified, and significant progress was made in characterizing and documenting the physical, chemical and structural properties of several of these coals. Facilities were designed and/or under construction for study of coal devolatilization, char oxidation, and in situ CARS study of flames. Development of submodels and collection of experimental data for SO_x removal and hazardous waste combustion were also initiated. Advanced chromatographic methods were developed for separation of and structural assignment to hydrocarbon fragments from coal extracts of six ACERC coals. Time-resolved Curie-point pyrolysis mass spectrometer studies of a Pittsburgh #8 coal revealed an aromatic distillable fraction, a long chain aliphatic hydrocarbon fraction showing thermoplastic degradation characteristics and a vitrinite-like phenolic fraction exhibiting thermosetting degradation behavior. A new solid state nuclear magnetic resonance spectroscopy technique was developed for aromatic ring structural analysis in coals.

Other accomplishments through the spring of 1987 included the hiring of center secretarial and administrative staff, design and production of a brochure, publication of internal and external newsletters, design and initial construction of new laboratories, and a campaign to increase industrial funding/participation. An educational (academic) program was organized to include new coursework, options, and fellowship programs in combustion-related areas at the two universities. An annual review meeting was held March 5-6, 1987, at BYU involving over one hundred participants from industry, government, academia, and the center. The initial response to the progress during the first year was generally enthusiastic. Thus, it appears that ACERC is off to a good start while combustion research is "heating up" at the BYU and the U of U campuses. □