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Development of a Coal Quality Expert™ A DOE Assessment

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Executive Summary

This document serves as the U.S. Department of Energy (DOE) post project assessment of the Clean Coal Technology (CCT) Round 1 project *Development of a Coal Quality Expert.* In 1990, CQ Inc., then a subsidiary of the Electric Power Research Institute (EPRI), and Combustion Engineering (now ABB Combustion Engineering, Inc.) executed a cooperative agreement with DOE. Both contractors became co-prime contractors for the project; project management and administrative duties were delegated to CQ Inc. Project participants included several contractors and utilities. The total project cost was $21.7 million, of which 50 percent was provided by DOE.

The goal was to deliver a software tool for utilities, coal producers, and equipment manufacturers that could analyze the impacts of coal quality, capital improvements, operational changes, and/or environmental compliance alternatives on power plant emissions, performance, and production costs. This software was named the Coal Quality Expert (CQE™). The project scope included supporting tasks: (1) to collect and analyze data to form the basis for CQE™ algorithms, methodologies, and submodels; and (2) to verify the accuracy and integrity of the software. Coal characterization, bench- and pilot-scale combustion testing, and full-scale utility demonstration tests as well as software development and demonstration tasks were included in the project.

Data from these activities were used to develop CQE™ algorithms and models. The utility boiler field test results were also correlated with EPRI's Coal Quality Impact Model (CQIM) predictions.

A CQE™ beta version was released in May 1995 and evaluated by several utilities by July 1995. Version 1.1 was released in June 1996. CQE™ has been distributed to about 25 utilities in the United States and one in the United Kingdom through membership in EPRI.

I Introduction

The goal of the U.S. Department of Energy (DOE) Clean Coal Technology (CCT) Program is to furnish the energy marketplace with advanced, more efficient, and environmentally responsive coal utilization technologies that have been developed beyond the proof-of-concept stage.

This document serves as a DOE post project assessment of a project in CCT Round 1, *Development of the Coal Quality Expert.* The project is described in a 1990 report to congress, which is listed in the bibliography at the end of this document. In June 1990, CQ Inc., then a subsidiary of the Electric Power Research Institute (EPRI), and Combustion Engineering (now ABB/CE) executed a cooperative agreement with DOE; CQ Inc. and ABB/CE became co-prime contractors for the project. Project management and administrative duties were delegated to CQ, Inc., which is now a privately held company. Total project cost was $21.7 million, of which 50 percent was provided by DOE. The work began on May 3, 1990, and was completed on June 30, 1996.

This independent evaluation is based on information from the CQ Inc. final report *Development of a Coal Quality Expert* (1998) and other reports. These reports are listed in the bibliography at the end of this document.

The Coal Quality Expert (CQE™) is a personal computer software package. This predictive tool helps coal-burning utilities select the economically optimum coal for a specific boiler, based on environmental emissions constraints, operational efficiency, performance limitations, and cost. The software predicts operating performance and associated costs of coals not previously burned at the facility. Data obtained from bench-, pilot-, and commercial-scale testing of selected coals were used to develop, adapt, and verify the algorithms in CQE™. Utility boiler field tests were performed at six sites. Two coals — the coal currently used as fuel was the baseline, and an alternate coal that was blended or cleaned to improve quality — were burned in the boilers over 2-month test periods.

The objective of this project was to develop and deliver a software tool that could:

- Improve upon EPRI's existing coal quality information system (CQIS) database and coal quality impact model (CQIM) to allow confident assessment of the effects of coal cleaning on specific boiler costs and performance.

- Make accurate and detailed predictions of coal quality impacts on total power plant capital cost, operating cost, and performance based on detailed coal quality information, without bench-, pilot-, or field-scale tests.

Beta testing of the CQE™ model was performed by several utilities in mid 1995 and the final version was released in June 1996. Under the terms of the cooperative agreement between DOE and the participants, DOE received the commercial version of CQE™, released in June 1996. DOE is to receive updates to the software as they become available.

II Technical and Environmental Assessment

II.A Promise of the Technology

The goal of this project was to develop a software product that could be used as a stand-alone workstation or as a network application by utilities, coal producers, and equipment manufacturers. The product was to analyze the impacts of coal quality, capital improvements, operational changes, and/or environmental compliance alternatives on power plant emissions, performance, and production costs.

The project involved (1) the characterization and cleanability analyses of various coals, (2) bench- and pilot-scale combustion testing of the coals in question, and (3) full-scale utility demonstration tests. Data obtained from these tests was intended to develop the algorithms, subroutines, and programs included as part of the CQE™ product. The relationship between these aspects of the project is shown in the process flow diagram, Figure 1.

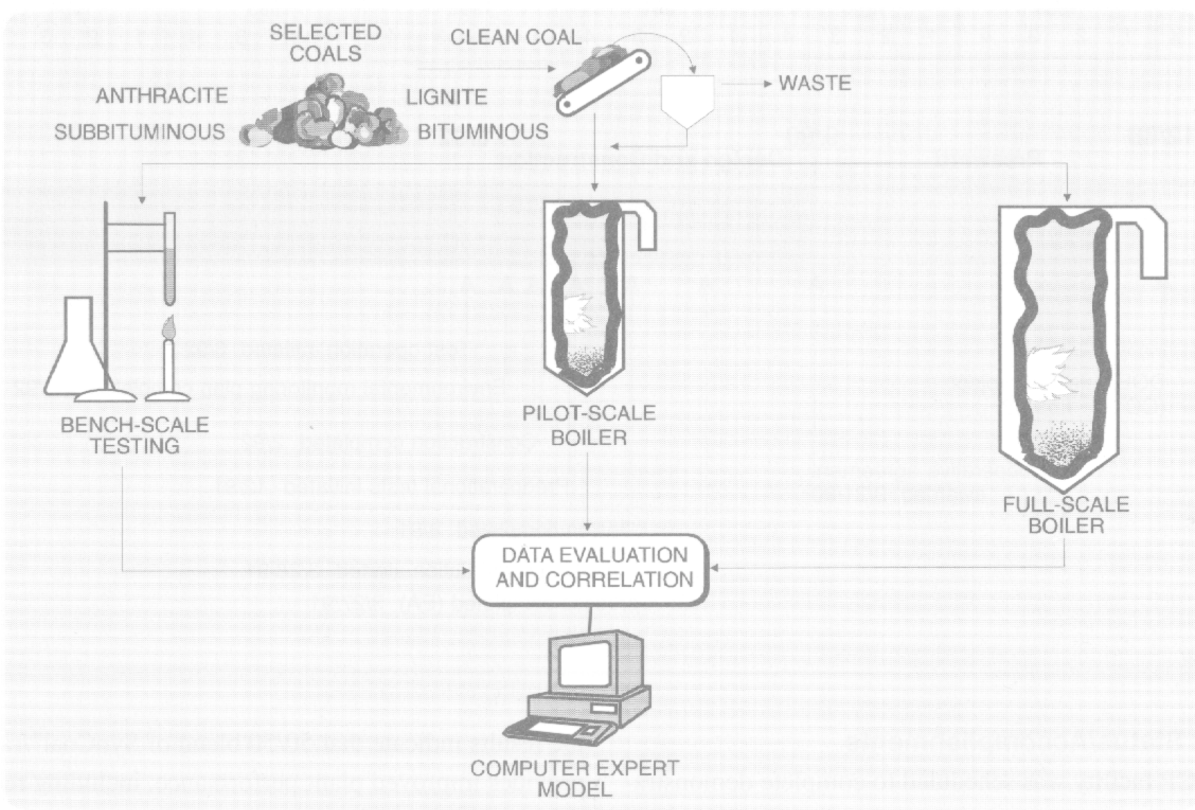

Figure 1. CQE Process Flow Diagram

The project was originally conceived to incorporate the results and products of several ongoing research and development (R&D) projects into computer software that would become a standard for studying fuel-related issues in the power industry. The CQE™ model, which addresses fuel quality from the coal mine to the busbar and the stack, is an integration of predecessor software tools. It was designed to answer critical questions that must be considered before a utility can be certain that it is operating its power plants within emissions limitations at the lowest possible cost.

The CQE™ software is composed of models that (1) evaluate performance issues; (2) examine emissions and regulatory issues; and (3) relate performance to costs, which include consumables (fuel, sorbents, etc.), waste disposal, and operation and maintenance.

Coal cleaning to remove sulfur and ash adds to the cost of the fuel, but can offer benefits in reduced operating costs. The economic impact of coal cleaning is shown schematically in Figure 2. CQE™ is designed to quantify these relationships, using commonly available coal quality information as input data.

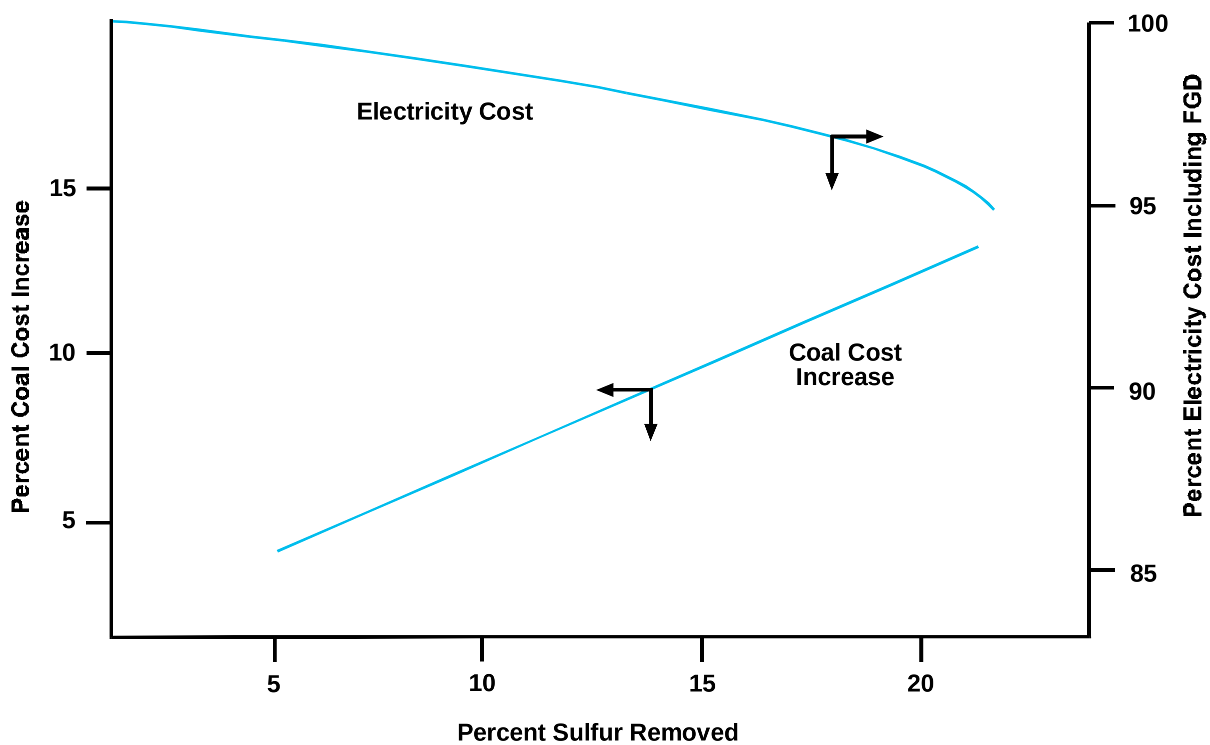

Figure 2. Economic Impact of Coal Cleaning

Figure 3 shows that traditional methods of evaluating coals for power plant use involve testing on a large scale over a considerable period of time. CQE™, however, permits the use of much smaller quantities of coal over significantly shorter time periods. By incorporating algorithms based on large amounts of available data, CQE™ can predict power plant performance by characterizing the fuel. Full-scale test burns are still recommended in instances where the alternate fuel quality differs significantly from the currently used coal. CQE™ can be used to screen alternate fuels for economic, environmental, and operational viability. Furthermore, CQE™ can be used to better manage the test burn, allowing operators to focus on areas of concern. Finally, CQE™ can be used to assess long-term operating impacts that may not be apparent during a short-term test.

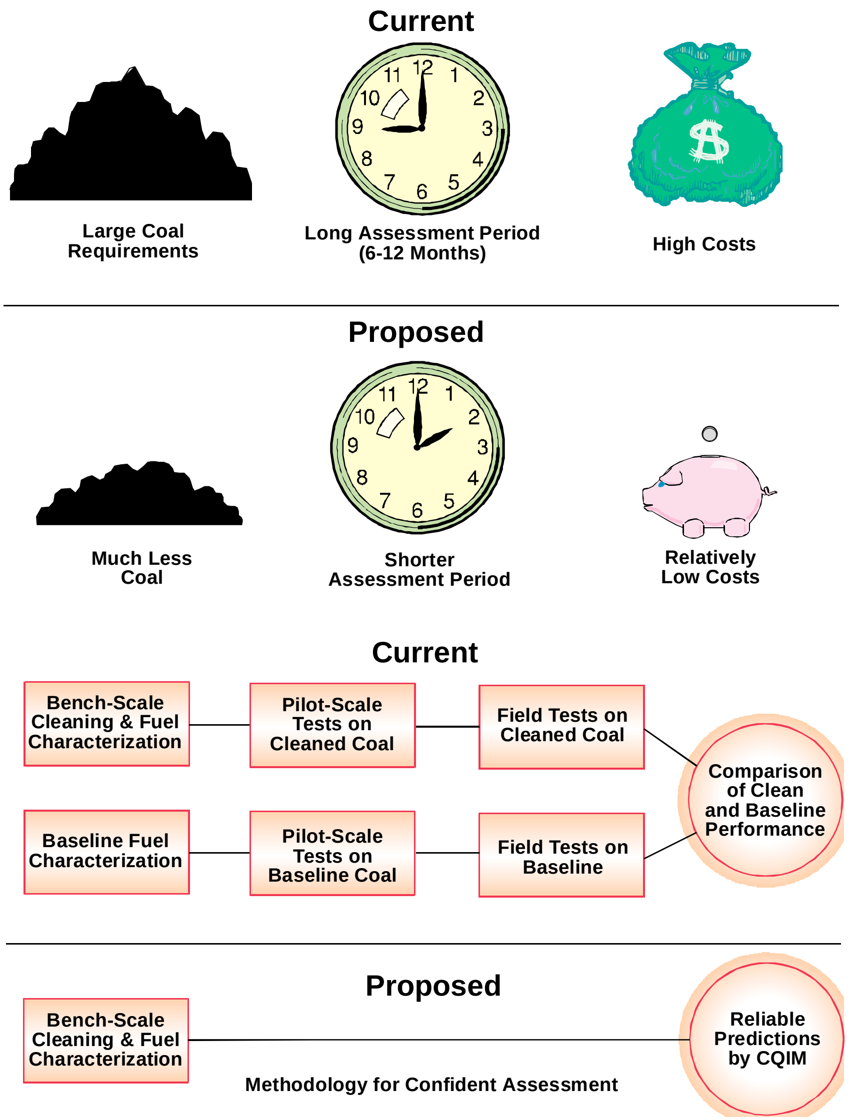

Figure 3. Comparison of Assessment Methods

II.B Project Description

The CQE™ design incorporated sophisticated modeling techniques, including object-oriented design and an object database management system. These techniques permit different views into the data, based on the specific situation being evaluated. CQE™ was also designed to be easy to use. The model uses roadmaps — pictorial representations of the steps to be completed in performing an analysis or evaluation — to ensure that all steps are completed and to illustrate the current status of the evaluation. Existing technology was also incorporated into the model to improve the overall results and ease of use. For example, CQE™ incorporated existing programs and data, including EPRI's CQIM and CQIS databases.

The CQE™ project included numerous supporting tasks (1) to collect and analyze the data that form the basis for the algorithms, methodologies, and submodels; and (2) to verify the accuracy of the relationships in the software. This effort drew upon the expertise of boiler designers, coal scientists, software specialists, coal cleaning experts, and boiler test teams and operators.

Coal Characterization Studies

CQ Inc. conducted 13 detailed coal cleanability characterization studies to provide baseline data for the CQE™ model. This step involved extensive investigations of physical and chemical properties of all components of the coal and assessments of the potential for removing ash-forming, sulfur-bearing, and trace element-bearing minerals associated with this coal. These coal characterizations were completed in conjunction with field combustion testing at four locations:

- Public Service of Oklahoma's (PSO) Northeastern Station
- Mississippi Power Company's (MPC) Jack Watson Station
- Northern States Power Company's (NSP) Allen S. King Station
- Alabama Power Company's (APC) Gaston Station

Combustion testing also was done at New England Power Company's (NEP) Brayton Point Station (two units), but coal characterizations were not performed in conjunction with those tests.

Pilot-Scale Combustion Tests

Pilot-scale combustion tests were conducted to support the coal cleanability characterization and field testing efforts. ABB/CE was responsible for all pilot-scale combustion tests with the exception of the cyclone boiler simulations, which were the responsibility of The Babcock & Wilcox Company (B&W). Four pilot-scale combustion test series were completed and each series included the following:

- Bench-scale fuel characterization
- Test furnace performance evaluation
- Data analysis and reporting

ABB/CE's Fireside Performance Test Facility (FPTF) and B&W's Small Boiler Simulator (SBS) were used to evaluate the effects of coal properties on pulverization, ash deposition, combustion, erosion, and emissions. The primary purpose was to provide data that can be used to predict full-scale boiler combustion performance from pilot-scale tests, while providing detailed quantitative performance data for CQE™ algorithm development.

Utility Boiler Field Tests

Boiler field testing was vital in establishing correlations between field-, pilot-, and bench-scale testing. Correlations for fouling and slagging sample analyses were of special interest. Comprehensive test burn evaluations were performed at six utility test sites. Testing at each site consisted of a baseline coal test, using the coal currently being burned at the unit, and an alternate coal test, in which a coal or coal blend of improved quality was evaluated. The utility boiler field test results were correlated with CQIM predictions and were used to develop and verify the CQE™ program.

II.C Project Objectives and Results

The objective was to develop and demonstrate an expert system that could be run on a personal computer. The system was to provide coal-burning utilities with a predictive tool to assist in selecting the optimum quality coal for a specific boiler, based on operational efficiency, cost, and environmental emissions. Data for the models to be included in the CQE™ program were obtained from bench-, pilot-, and full-scale tests as well as from EPRI and open literature. The final product is not a true expert system, but is a tool for providing rational selection of fuels.

All six of the proposed field tests were completed and a CQE™ prototype model was showcased in 1993. Final model development and verification were performed in 1994 and a CQE™ alpha version was released in March 1995. A beta version was released in June 1995 and Version 1.1 was released in June 1996.

CQE™ consists of several sub-models that exist in formats that are compatible with other software. The sub-models are described in the following paragraphs. Some of these codes and models were developed by EPRI (sometimes with DOE support) as part of other programs and were not the focus of the CQE™ project.

Coal Quality Impact Model (CQIM): CQE™ uses the core of the CQIM code to evaluate the impacts of coal quality on performance of coal-fired power plants. The CQIM code also can be used to perform maintenance/availability, derating, sensitivity, and economic analyses**.**

Model Constructor: Model Constructor builds on CQIM's graphical representation of a unit's configuration. It represents the physical layout of the unit, graphically building the power plant model. The user selects components from a toolbar that represents the individual equipment systems and then connects the air, fuel, and flue gas flow through the unit. The user can easily verify the accuracy of the model layout and can review the models used to understand the unit layout.

Acid Rain Advisor (ARA): ARA was developed as part of the CQE™ project. The user can rapidly select combinations of sulfur dioxide (SO_2) reduction technologies for various units in a system, while viewing system-wide results. The purpose of this model is to help the user evaluate options for compliance with the Clean Air Act Amendments (CAAA) of 1990. ARA can be used on a stand-alone basis, in conjunction with CQIM, or within CQE™. It was released in 1992 for utilities to use while preparing CAAA compliance plans, well before the release of CQE™.

CQE™ software incorporates an advanced boiler model set, which consists of the SLAGGO and FOULER routines developed by PSI PowerServe and the University of North Dakota Energy and Environmental Research Center. The CQE™ design expands boiler performance modeling beyond CQIM capabilities to interface with and use results from these routines to predict deposit growth and strength, soot blower schedule, and soot blower effectiveness. SLAGGO and FOULER offer an improved approach to and significant technical advantages in modeling the impacts of coal quality on power plant emissions, but they were never completely verified. Thus, they should be considered research codes.

- **Slagging Expert (SLAGGO):** SLAGGO simulates the coal combustion cycle of ash formation, deposit initiation, growth, and removal, based on coal properties, boiler design, and operating parameters. SLAGGO consists of several models and submodels: ash formation, ash transport, deposit growth, thermal properties, and deposit removal models; and mineral matter transformation, alkali vaporization, and excluded pyrite kinetics submodels. Coal properties, boiler internal aerodynamics, and transport mechanics are accounted for to predict any change in cleanliness of the waterwall and superheater tubes in the furnace. Deposit removal by soot-blowing is also modeled.

- **Fouling Expert (FOULER):** FOULER predicts convective pass fouling, based on boiler design, temperature and gas distributions, ash size and composition distributions, and soot-blowing and load drop parameters. The thermal resistivities of each heat exchange section are used to iteratively calculate boiler temperature profiles, and a cleanliness factor is determined from the difference in heat transfer between dirty and clean tubes. Time intervals between soot-blowing cycles can be optimized with FOULER.

- **Coal Cleaning Export:** This model evaluates various cleaning processes and predicts the cost of cleaning facilities, based on a production quantity and quality specified. This information is compared with other emissions reduction options to determine the best economic option.

II.D Environmental Performance

Calculation routines were deployed to estimate environmental emissions as a function of fuel, boiler, and plant operation. In addition, the CQE™ project was subject to DOE compliance procedures, and an approved environmental monitoring plan (EMP) was prepared covering all six utility field test sites. Environmental monitoring reports (EMRs) were prepared during the project and a final EMR was prepared for each field test site.

II.E Post-Project Achievements

The CQE™ program has been made available to EPRI member utilities and is operational. Further refinement of the algorithms and input/output techniques will be performed as continued use is made of the program. Three products are available: use licenses, consultant licenses, and commercialization licenses.

A users group was established, and a CQE™ homepage was created on the internet (http://147.182.5.102/cqe/cqe.htm) to promote the software, facilitate communication with and among users, and distribute an on-line user's manual. An update of CQE™, Version 1.1, was issued in June 1996.

III Operating Capabilities Demonstrated

III.A Coal Characterization

The CQ Inc. final report gives the characteristics of each coal tested and the potential for improving coal quality using coal cleaning techniques and trace element reduction during coal cleaning. Significant quantities of data are presented along with discussion of the fouling/slagging potential of the cleaned coal and the energy recovery.

III.B Pilot-Scale Combustion Tests

Pilot combustion tests were conducted to support the coal cleanability characterization and field testing efforts. Fifteen different coals or coal blends from six different power plants were tested in ABB/CE's FPTF and B&W's SBS. The purpose of this phase of the work was to be able to predict full-scale boiler combustion performance from pilot-scale tests and to provide detailed quantitative performance data for CQE™ algorithm development.

The final report summarizes the tests made in each facility using each of the coals or coal blends. Included is an example fuel evaluation, involving comparison of an eastern high sulfur coal, an Illinois Basin coal, and a Powder River Basin coal. Output includes the technical and economic performance of each coal. In this particular example, the Powder River Basin coal was the best fuel choice on the basis of performance and cost.

As an example of a fuel evaluation conducted in this project, the final report includes results for pilot- and bench-scale testing of Wyoming (WY), Oklahoma (OK), and blends of WY and OK coals at PSO's Northeastern Unit 4. These results indicate that if only the viscosity of the deposits is considered, the ranking of deposit severity was, worst to best:

- 90 WY/10 OK
- 100 WY
- 70 WY/30 OK (cleaned)
- 70 WY/30 OK

Also, indicated was heat-flux recovery after soot-blowing. Again, from worst to best:

- 100 WY
- 70 WY/30 OK
- 90 WY/10 OK
- 70 WY/30 OK (cleaned)

The results for MPC Watson Unit 4 indicate that the baseline coals, Illinois No. 2, 3, and 5, had better slagging performance than the alternate coal, Kentucky No. 11, but the fouling performance was similar. Results from the pilot-scale tests also indicated that the alternate coal produced more low-viscosity liquid phase material, confirming the full-scale test results, which showed the alternate coal to have a higher slagging propensity than the baseline coal. Analysis also indicated that more severe fouling could occur during combustion of the alternate coal than the baseline coal.

The NSP King Unit 1 tests were performed in a pilot-scale cyclone furnace at B&W's Alliance Research Center, feeding WY, Montana (MT), and petroleum coke (PC). Unlike the full-scale unit, the feed coals were pulverized because of the small size of the cyclone. The results indicate that the baseline coal, 70 WY/20 MT/10 PC, had a medium to high slagging potential and a low to medium fouling potential. When compared to the alternate coal, 93 WY/7 PC, the furnace exit gas temperature (FEGT) of the baseline coal was 25 °F higher, nitrogen oxides (NO_X) emissions were 50 ppm lower, and SO_2 emissions were 100 ppm higher. Both coals exhibited good heat flux recovery after soot-blowing.

III.C Utility Boiler Field Tests

Comprehensive test burn evaluations were performed at six utility test sites:

- PSO's Northeastern Unit 4
- MPC's Plant Watson Unit 4
- NSP's King Unit 1
- APC's Gaston Unit 5
- NEP's Brayton Point Units 2
- NEP's Brayton Point Units 3

At each facility, a baseline coal and an alternate coal were tested. The CQE™ field test program was divided into several major activities. Diagnostic tests were conducted at the start of the test program to determine if the unit was operating at expected performance levels. The unit was then tested with the baseline coal, followed by testing of the alternate coal. Three-day characterization tests were conducted, which included detailed evaluations of pulverizers, boiler, and precipitator performance.

In addition, the tests included special instrumentation to measure gas temperature in the lower furnace region of the boiler, low-temperature flue-gas corrosion at the air preheater outlet, and fouling rates of the convective sections of the boiler.

Six CQIMs, one for each boiler tested, were developed during the project and run with the baseline and alternate coals. The main objectives of the CQIM validation efforts were to:

- Evaluate the accuracy of CQIM predictions versus test data.

- Assess the benefits of calibrating CQIM using detailed test burn data.

- Identify elements of the CQIM predictions in which test burn results of improved equipment models could be used to enhance the predictive capabilities of CQIM and CQE™.

The final report lists results and conclusions from the field tests, including relative slagging/fouling rates for baseline and alternate coals, soot-blowing requirements, and FEGT, pulverizer performance, and particulate removal performance information. Although coal cleaning is a key ingredient of strategies for improved coal utilization, the CQE™ model addresses a wide range of factors involved in power generation from coal. Therefore the report focuses on overall model capability rather than providing detailed results of coal cleaning.

III.D Environmental Monitoring

As a CCT project, CQE™ was subject to DOE compliance procedures. An EMP was prepared for all six utility field tests. Both compliance and supplemental monitoring were conducted during the field tests to satisfy the requirements of the EMP. In addition, EMRs were prepared during the project and a final EMR was prepared for each field test site.

EMR results are summarized in the final report. Both baseline and alternate fuels were tested, and occasional excess opacity levels were observed in one or more of the tests. No NO_X or SO_2 emissions standards were exceeded, although the higher sulfur alternate coal at the MPC Watson Unit 4 site had 5 percent higher SO_2 emissions than the baseline coal.

III.E Commercialization of the Technology

The ARA software became available in 1992, and two commercial sales were made, one in 1993 and one in 1995. Debugging of the CQE™ software proceeded through the end of the project. A beta version was released in May 1995 and evaluated by several utilities by July 1995. The initial commercial version was released in December 1995, and an updated Version 1.1 was issued in June 1996. CQE™ has been distributed to about 25 utilities in the United States and one in the United Kingdom through membership in EPRI. Black & Veatch (B&V) executed the first CQE™ commercialization license, and CQ Inc. is also licensed to commercialize CQE™. Under the terms of that license, B&V and CQ Inc. are working in an independent, but confidential, manner to sell use and consulting licenses worldwide.

IV Market Analysis

IV.A Product Advantages

Given its array of capabilities, CQE™ has significant commercial value for use by power generation companies, equipment manufacturers, environmental assessment firms, litigators, fuel suppliers, government organizations, and engineering firms. Three separate products exist for CQE™: use licenses, consultant licenses, and commercialization licenses.

CQE™ can predict power-plant performance with a minimum number of bench-scale tests. This means the desired assessments can be achieved at a much lower cost than using traditional approaches. Users will have to balance these savings against the cost of a CQE™ software license. The final report does not include proprietary information on the algorithms that were developed for incorporation into the model.

IV.B Potential Problems

Factors adversely affecting CQE™ model sales, recognized by CQ Inc., include: (1) EPRI members receive the model as part of their dues whereas outside firms have to pay a relatively high purchase price, (2) competition from in-house programs, and (3) a language barrier — the software is written for the OS/2 operating system.

V Conclusions

Development of the CQE™ model included a large number of bench-scale coal characterization tests, pilot-scale combustion tests, and full-scale utility boiler field tests. The resulting CQE™ software offers significant benefits in selecting coal-based fuels and designing and operating coal-fired power systems. By incorporating algorithms based on available data, CQE™ can predict power-plant performance with a minimum number of cleanability and fuel characterization bench-scale tests. The net result should be a much lower cost to achieve the desired assessments compared with traditional approaches.

The coal characterization tests performed in this study measured the effectiveness of physical coal cleaning in removing ash-forming minerals, pyritic sulfur, and trace elements from bituminous and subbituminous coals. Pilot-scale combustion tests and utility boiler field tests helped characterize the combustion of coals that improve environmental impacts over pre-project choices made by the utilities involved in this evaluation. This project provided invaluable information to all project participants, including six utilities. The six utilities benefitted by obtaining:

- Practical boiler tuning, resulting in improved day-to-day operating efficiency and reduced emissions.
- Expert advice on boiler operation using the baseline coal and the alternate coal.
- Practical experience in burning an alternate coal chosen for improved environmental performance compared to the utility's coal of choice.

The ARA software, developed as part of the CQE™ project, can be used to select CAAA compliance strategies, either within CQE™ or as a stand-alone program.

VI Abbreviations

APC	Alabama Power Company
ARA	acid rain advisor
B&V	Black & Veatch
B&W	The Babcock & Wilcox Company
CAAA	Clean Air Act Amendments of 1990
CCT	Clean Coal Technology (program)
CQE™	Coal Quality Expert
CQIM	Coal Quality Impact Model
CQIS	Coal Quality Information System
DOE	U.S. Department of Energy
EMP	environmental monitoring plan
EMR	environmental monitoring report
EPRI	Electric Power Research Institute
FEGT	furnace exit gas temperature
FOULER	fouling expert (research code)
FPTF	Fireside Performance Test Facility
MPC	Mississippi Power Company
MT	Montana (coal)
NEP	New England Power Company
NO_X	nitrogen oxides
NSP	Northern States Power Company
OK	Oklahoma (coal)
PC	petroleum coke
PSO	Public Service of Oklahoma
R&D	research and development
SBS	Small Boiler Simulator
SLAGGO	slagging expert (research code)
SO_2	sulfur dioxide
WY	Wyoming (coal)

VII Bibliography

Combustion Engineering, Inc., and CQ Inc. 1990. *Development of the Coal Quality Expert,* Comprehensive Report to Congress, Clean Coal Technology Program, proposed by Combustion Engineering, Inc. and CQ Inc.

CQ Inc. 1998. *Development of a Coal Quality Expert*, Final Report.

Harrison, C.D. 1992. Coal Quality Expert: Status and Software Specifications, presented at the First Annual Clean Coal Technology Conference, Cleveland, Ohio, November 1992.

Harrison, C.D., D.B. Kehoe, D.C. O'Connor, and G.S. Stallard. 1995. CQE: Integrating Fuel Decisions, presented at the Fourth Annual Clean Coal Technology Conference, Denver, Colorado, September 1995.

Harrison, C.D., D.B. Kehoe, D.C. O'Connor, and G.S. Stallard. 1997. Recent Experience with the CQE™, presented at the Fifth Annual Clean Coal Technology Conference, Tampa, Florida, January 1997.

O'Connor, D.C. 1994. The CQE Project: Producing Innovative Software for Economical Deployment of Coal Technologies, presented at the Third Annual Clean Coal Technology Conference, Chicago, Illinois, September 1994.

U.S. Department of Energy. 1997. Development of the Coal Quality Expert™, *U.S. Department of Energy, Clean Coal Technology Demonstration Program - Program Update*, p.5-116, October 1997.

U.S. Department of Energy. 1996. CQ Inc. Software Tool Eases Utility Decision-Making, *Clean Coal Today*, issue 23, Fall 1996.