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**Modeling of Integrated Environmental
Control Systems for
Coal-Fired Power Plants**

Technical Progress Report

To

**Pittsburgh Energy Technology Center
U.S. Department of Energy
Pittsburgh, Pennsylvania 15236**

From

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MS **MASTER**

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1 INTRODUCTION

This is the first quarterly report of DOE/PETC Contract No. DE-AC22-87PC79864, entitled, "Modeling of Integrated Environmental Control Systems for Coal-Fired Power Plants." The report covers accomplishments through the period ending December 31, 1987.

During this time efforts were devoted principally to the first Work Statement task, which was the definition of a revised and detailed work plan for the remaining project effort. A kickoff meeting with DOE/PETC personnel was held in November 1987 at which the revised work plan was presented and reviewed. The final plan was submitted to DOE in December 1987, and is presented here as a key accomplishment of the preceeding quarter.

2 DETAILED PROJECT WORK PLAN

This section presents a detailed work plan corresponding to Task 1 of the contract Statement of Work. The four remaining tasks are discussed and a timetable for scheduled deliverables is developed.

Table 1 shows the overall level of effort available for this project over the 36-month period of performance. A total of 41.7 man-months is available. The allocation of this effort to each of the principal work statement tasks also is shown in the table.

Table 2 summarizes the proposed schedule of milestones and deliverables for each task. The following sections presents a work breakdown structure for each of these tasks, elaborating on the research to be performed and the results expected.

Table 1

MODELING OF INTEGRATED ENVIRONMENTAL
CONTROL SYSTEMS FOR COAL-FIRED POWER PLANTS

Project Effort (36 mos):

Principal Investigator	5.7 mos
Research Associate	18.0 mos
Graduate Assistant	18.0 mos
<hr/>	
TOTAL (man-mos)	41.7

Project Tasks:

Effort (man-mos)

1. Develop Detailed Work Plan	0.7
2. Refine Existing Models	12.0
3. Model New Processes	9.0
4. Conduct Case Studies	3.0
5. Document and Transfer Model	17.0

Table 2

PROPOSED PROJECT TIMETABLE AND DELIVERABLES

▲ Signifies a project deliverable.

2.1 Task 2: Refine Current Models

This task involves refining and updating models for several technologies in the Integrated Environmental Control (IEC) model developed in an earlier DOE project (DE-FG22-83PC60271). Table 3 highlights some of the accomplishments of this previous project.

Table 4 summarizes the technologies to be refined as part of this task. Our work on pre-combustion control technology will focus on, (1) the addition of a froth flotation circuit to the current model of conventional coal cleaning plants, and (2) extension of the current heavy media separation circuit to treat coals of finer sizes (100-150 mesh). Technical performance and cost data for these enhancements will be obtained from DOE sources and incorporated into the IEC model.

Additional refinements to three post-combustion control technologies for combined SO_2/NO_x removal also are part of this task. Enhancements to the fluidized bed copper oxide process model will include consideration of alternative regeneration gases, process impacts on air preheater performance, and a more detailed model of the sulfur recovery plant.

Improvements to the NOXSO process model also will include systematic treatment of the sulfur recovery system, as well as the coupling between NO_x and SO_2 removal. Recent data on sorbent attrition rates and NO_x reduction efficiency also will be incorporated.

For the electron beam process, experimental data from recent laboratory and field tests will be used to improve the existing models of process performance for SO_2 and NO_x removal as a function of dose and other key system parameters. Algorithms developed by Research Cottrell and/or Ebara, Inc. will be used for this purpose.

During the course of this task, additional efforts to upgrade existing models of "conventional" flue gas treatment technologies (SCR, FGD, particulate collectors

Table 3

ACCOMPLISHMENTS OF PREVIOUS DOE PROJECT

- Developed new computerized framework for evaluating IEC system performance and cost
 - Deterministic analysis
 - Probabilistic analysis
- Developed and implemented models of conventional and advanced processes for environmental control:
 - Conventional coal preparation (4 levels)
 - Coal-pyrite floatation process
 - High gradient magnetic separation
 - Selective catalytic reduction
 - Wet limestone FGD system
 - Lime spray dryer FGD system
 - Electrostatic precipitator
 - Fabric filter collector
 - Solid waste disposal
 - Electron beam process
 - Fluidized bed copper oxide process
 - NOXSO process
- Conducted case studies illustrating role of advanced technologies and integrated systems
- Delivered final report documenting all results and derivation of process models

Table 4

TASK 2:

REFINE EXISTING MODELS OF
PERFORMANCE AND COST

- ° Conventional Coal Cleaning
 - Add optional froth floatation circuit
 - Extend dense media vessel to finer coals
 - Develop associated economics models
- ° Copper Oxide Process
 - Include alternative regeneration methods
 - Include impact on air preheater performance
 - Add sulfur recovery system model
 - Update process economics model
- ° NOXSO Process
 - Add coupling of SO_2 and NO_x removal rates
 - Add sulfur recovery system model
 - Update process design details
 - Update process economics model
- ° Electron Beam Process
 - Update SO_2/NO_x performance models
 - Update process economics model

and solid waste handling) also may be necessary and/or desirable since these technologies also are still evolving. Such efforts will be discussed with the DOE project officer and added to the work scope if warranted.

The deliverables from this task will be a series of technical reports documenting the improvements that were made. The schedule for these reports appears in Table 2.

2.2 Task 3: New Process Models

This task involves developing and implementing analytical models of several new control technologies, with emphasis on advanced coal cleaning processes. Table 5 summarizes the new options to be included. Advanced flotation methods using microbubbles will be one of the technologies modeled. True heavy media separation and selective agglomeration processes also will be modeled. Characterization of performance and cost will be based on studies available from DOE contractors during the course of this project.

To the extent that time is available we will also develop models of one or more new combustion and/or post-combustion control technologies, such as furnace or duct sorbent injection. This will depend largely on the priority given in Task 2 to upgrading the models of conventional post-combustion technologies, which was not part of the original work plan for this project. Developments in Europe and Japan during the past year, however, have changed the outlook for the "baseline" technologies to which advanced systems must be compared. Thus, it appears prudent to re-direct some project effort to insure that such developments are reflected in the IEC framework.

The deliverables under this task will be a series of technical reports documenting all aspects of the work. The timetable for this appears in Table 2.

Table 5

TASK 3:
DEVELOP PERFORMANCE AND COST MODELS
FOR NEW PROCESSES

- Advanced Coal Cleaning Processes
 - Heavy liquid cyclones
 - Selective agglomeration
 - Microbubble floatation
- Post-Combustion SO_2/NO_x Processes
 - Duct injection system, or
 - Other new/retrofit technology

2.3 Task 4: Case Studies

This task will involve exercising the IEC model in a series of case studies aimed at illustrating applications of the model to R&D planning and the identification of cost-effective environmental control strategies using IEC concepts. Table 6 summarizes the activities under this task. All of these will highlight the unique capability of the IEC model to perform probabilistic analysis. The deliverables (Table 2) will be a series of technical reports summarizing results of these analyses.

2.4 Task 5: Documentation and Transfer

This task involves, (1) the preparation of two kinds of written documentation for the IEC model, (2) delivery of the model to DOE, and (3) initial efforts on an interactive menu system for "user-friendly" operation of the model. These activities are summarized in Table 7.

Model documentation will consist of (1) analytical documentation describing the technical basis and development of all new or enhanced technology models, and (2) computer documentation describing the operation of the IEC model for an experienced computer operator. The latter effort will assume (require) that the model operator be familiar with the Demos command language in which the IEC model is implemented. A Demos User's Manual will be provided along with an operator's manual for the IEC model.

To facilitate use of the IEC model by less experienced operators, we will begin development of an interactive software system using "menus" and an advanced window manager. This will allow IEC systems to be configured and analyzed with a minimum of effort. Progress on the development of a more "user-friendly" system, however, will depend strongly on the availability of additional technology transfer support being sought to supplement the current DOE effort.

The choice of computer hardware for the model also will affect the effort on this task to some degree. Table 8 summarizes the available options. Our

Table 6

TASK 4:
CASE STUDIES AND APPLICATIONS

- Deterministic and Probabilistic Analyses
- Elicitation of Expert Judgments
- Applications to Research Planning and Management
- Identify Optimum Design Configurations
- Cost-Effectiveness of Integrated Process Designs
- Comparisons with Conventional Technologies

Table 7

TASK 5:
MODEL DOCUMENTATION AND TRANSFER

- Analytical Documentation
 - All new process performance models
 - All new process economic models
- Computer Model Documentation
 - Plant, economic and process models
 - Loading the model
 - Displaying parameters and variables
 - Basic Demos structure and commands
 - Deterministic analysis
 - Probabilistic analysis and graphing
 - Re-defining variables
 - Exiting and saving the model
- Transfer to DOE
 - Hardware/software options
- Improved User Interfaces

Table 8

COMPUTER OPTIONS FOR MODEL TRANSFER TO DOE

Configuration	1	2	3	4	5	6
Machine	Sun 3/52	MacII	VaxII	IBM-RT	(Any)	VAX
Operating System	Unix	Macintosh	Unix	Unix	Unix	VMS
Window Manager	Andrew	Macintosh	Andrew	Andrew	X	DEC
Ease of Transfer	Easy	Easy	Easy	Uncertain	Difficult	Painful
Effort Needed	None	Modify Demos	Find/fix System bug	Find a Suitable Computer	Rewrite ICEZ	Rewrite Demos +ICEZ

recommendation is to transfer the IEC model to DOE on either a Sun 3/50 or Macintosh II advanced workstation. The former represents the current configuration at CMU. The latter option is currently being developed at CMU to support the Demos software in an environment more amenable to user-friendly interaction (including advanced graphics and menu systems).

Other workstations (Vaxstation and IBM-RT) also are available, but at significantly higher cost and with some remaining operability problems. The option of running the model on DOE's current VAX computers is precluded by the lack of a Unix operating system. As noted in our original proposal, most DOE machines use the VMS operating system. To operate on VMS, a substantial effort beyond the provisions of this project would be required to re-write all of the code underlying the IEC model.

Selection of the most suitable hardware will be made by DOE in consultation with CMU during the first year of the project. Transfer of the model to DOE will then take place halfway into the project (see Table 2). This will allow sufficient time to test and improve the software and associated documentation during the final phases of the project.

A schedule of deliverables for all analytical and computer documentation also appears in Table 2. The project will culminate in a final report summarizing all accomplishments.

3 OTHER ACCOMPLISHMENTS

Other activities initiated during the first quarter included work on (1) two combined SO_2/NO_x processes, (2) model documentation, and (3) the development of a draft framework for a computer menu system to facilitate use of the IEC model. These activities are briefly summarized below.

3.1 Combined SO₂/NO_x Processes

As indicated in the project work plan, additional research efforts are needed to insure that advanced processes for combined SO₂/NO_x removal are treated in a systematic and comprehensive fashion. Work has begun to develop and incorporate models of an air preheater and sulfur recovery plant for the copper oxide process. The sulfur recovery plant model will later be extended to the NOXSO process. Progress on these new model developments will be reported in the next quarterly report, by which time those models will have been developed and implemented.

3.2 Model Documentation

Documentation of the IEC computer model is being developed to accompany the eventual transfer of the code to DOE/PETC. In contrast to the technical documentation prepared as part of the earlier project, this effort involves developing a User's Manual for the actual computer program. A Table of Contents for the Manual has been drafted, along with several introductory sections. A complete draft of the manual is scheduled for completion in mid-1988.

3.3 Model Menu System

To facilitate wider use of the IEC model, we proposed to begin development of an automated menu system that would allow users to choose options and run the IEC model without recourse to the computer command language now needed to operate the model. As noted earlier, the complete implementation of such an effort will require resources beyond the scope of the present project. However, we have begun to develop a framework in which initial progress can be made toward this goal.

Figure 1 shows a schematic of a menu system that would include a tutorial on model operation, documentation of model components, and a series of menus for model operation. The model documentation now being written would fit directly into this framework, including the tutorial on model operation. A limited set of

Figure 1. Draft Schematic of a Menu System.

menus and commands for executing the model will be developed later in the project to demonstrate its capabilities. This would allow DOE/PETC to evaluate the merits of additional support for this activity.

4 CONCLUSION

During the course of this project we hope to work actively with process developers and potential model users to demonstrate the applications of the model to research planning and analysis. Progress in this effort will be summarized in the next quarterly report along with technical accomplishments on the four project tasks.

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