DOE/PC/89908--T3

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QUARTERLY TECHNICAL PROGRESS REPORT NO. 4

JULY - SEPTEMBER 1990

ENGINEERING DESIGN AND ANALYSIS OF ADVANCED PHYSICAL FINE
COAL CLEANING TECHNOLOGIES

for

U.S. DEPARTMENT OF ENERGY
PITTSBURGH ENERGY TECHNOLOGY CENTER
PITTSBURGH, PA

CONTRACT NO. DE-AC22-89PC89908

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October 20, 1990

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1.0 INTRODUCTION

This project is sponsored by the United States Department of Energy (DOE) for the "Engineering Design and Analysis of Advanced Physical Fine Coal Cleaning Technologies". The major goal is to provide the simulation tools for modeling both conventional and advanced coal cleaning technologies. This DOE project is part of a major research initiative by the Pittsburgh Energy Technology Center (PETC) aimed at advancing three advanced coal cleaning technologies - heavy-liquid cycloning, selective agglomeration, and advanced froth flotation through the proof-of-concept (POC) level.

The commercially available ASPEN PLUS process simulation package will be extended to handle coal cleaning applications. Algorithms for predicting the process performance, equipment size, and flowsheet economics of commercial coal cleaning devices and related ancillary equipment will be incorporated into the coal cleaning simulator.

This report is submitted to document the progress of Aspen Technology, Inc. (AspenTech), its contractor, ICF Kaiser Engineers, Inc., (ICF KE) and CQ Inc., a subcontractor to ICF KE, for the fourth quarterly reporting period, July through September 1990. ICF KE is providing coal preparation consulting and processing engineering services in this work and they are responsible for recommending the design of models to represent conventional coal cleaning equipment and costing of these models.

2.0 ADMINISTRATIVE ITEMS

AspenTech, along with its subcontractors, ICF KE and CQ Inc., participated in a project review meeting with DOE on August 7-8, 1990 at the DOE Contractor's Review Meeting in Pittsburgh. ICF KE also attended a UCB meeting concerning filling data gaps for conventional froth flotation on August 8.

AspenTech, along with its subcontractors, ICF KE and CQ Inc., presented a paper describing this modeling work at the DOE Contractors Conference in Pittsburgh on August 89, 1990.

During this work period, many items were completed as scheduled according to the plan of work. Several project items remain behind schedule due to interruptions in our work schedule and difficulties encountered in performing several work items. Both AspenTech and its subcontractor have allocated more personnel and resources on the project to help meet scheduled deadlines.

3.0 TASK 1.2 - ENGINEERING ANALYSIS OF CONVENTIONAL COARSE COAL CLEANING

3.1 Planned Scope of Work

The work plan for the fourth quarter of the project called for completion of the washability interpolation routine, gravity separation models, and dewatering models. As these items were completed, work in the areas of size reduction, classification and froth flotation were scheduled to begin. Topical reports for each completed category were to be submitted for each model category. As each model was completed, testing and validation procedures were scheduled to begin.

Costing models were also planned to be implemented and tested as each of the gravity separation models were completed.

3.2 Technical Status

The technical status of the interpolation routine, gravity separation models, dewatering models, froth flotation and miscellaneous items are discussed in the following sections.

3.2.1 Interpolation Routine

During the third quarter, no progress was made in correcting the problems associated with the washability interpolation program. Discussions with Dr. Peter Luckie, however, have identified the problem areas in the program along with suggested corrective action to be taken. For example, it is believed that the interpolation of cumulative attribute units (float) rather than cumulative attribute values within a gravity interval and over the entire size range will rectify problems associated with the interpolation of attributes.

ICF KE recognizes the importance of the interpolation routine to the success of the project and intends to complete this work within the fifth quarter.

3.2.2 Gravity Separation Models

During the work period, efforts were directed toward completing the suite of gravity separation models to be provided under the contract. Specifically, work was directed in the areas of developing the validity logic for each gravity

separation device; resolving data regression inconsistencies for dp and Ep relationships; resolving dp and Ep estimates for calculated composites using the spline routine; and completing the water split and equipment sizing algorithm programming for several gravity separation devices. Additionally, efforts were expended in testing and debugging the completed coarse coal jig, heavy media vessel, heavy-media cyclone and concentrating model programs. This exercise involved running the completed model over a desired range of operating conditions and checking the outputs for accuracy and completeness.

The development of validity ranges for each model entails statements to warn the user of his use of the model outside of the range of application and/or physical limitation on the gravity separation device. For example, for a coarse coal jig, the following validity checks have been incorporated into the program:

- Maximum coal feed size should be less than 8 inches. Typically, coarse coal jig feed is 4-5 inches or less in size.
- The range of dp value possible in this device should lie between 1.50 and 2.00.
- The maximum amount of near gravity material in the feed should not exceed 25 percent.

Data found in RI8238 for Ep and dp versus particle size was regressed into equations using a newly acquired statistical software package (MINITAB). MINITAB easily allows for the regression of data into polynomials and also accommodates situations where transformations (log, natural log, exponential, negative reciprocal, square root, etc.) may be used. Using available data, new equations relating Ep and dp versus particle size were determined for the coarse coal jig, heavy media vessel, heavy media cyclone, and concentrating table.

A problem encountered during coarse coal jig and heavy media vessel model development was the technique utilized for estimating dp and Ep for the summed composite. In the algorithm, the separation of solids is determined for each size interval followed by an overall composite calculation to determine the overall fractional recovery values for the composite feed. These values are then read into a cubic spline interpolation routine for determining spline coefficients and subsequently

estimating the specific gravity value at 50 percent recovery (overall dp). This estimated dp value is compared to the user requested dp value and the calculation sequence is repeated until the values are plus or minus 0.004 sq. gr. units apart. When the complete set of fractional recovery values are passed into the spline routine, inconsistent estimates of dp are observed and hence, influence the effectiveness of the convergence algorithm. However, if the fractional recovery values are first sorted to allow values only between 90 and 10 percent recovery, the spline estimates of dp, d_{25} AND d_{75} are adequate for the accuracy of the program in most cases (the spline routine is not accurate for sharp separations, see discussion later in text). The latter two values are used for calculating the composite Ep value.

Programming was completed for determining the water split and equipment size in the coarse coal jig, heavy media vessel, heavy media cyclone and concentrating table models.

Each model was subsequently tested for accuracy and completeness. For example, the coarse coal jig model was tested over an entire range of dp values from 1.50 to 2.00 by 0.01 increments. The resulting calculations were checked per the following criteria:

- The user dp value was successfully converged upon.
- Steadily increasing estimated Ep values with increasing dp.
- Appropriateness of composite Ep.
- Increasing clean coal yield with increasing dp.
- Decreasing clean coal quality as yield and dp increase.
- Completeness of all reports and calculations.
- Accuracy of water balance calculations.

The coarse coal jig model was also tested over a selected range of jig feed capacities ranging from 50 to 2,000 tons per hour. The results of these calculations were examined for accuracy in selecting the appropriate jig size and number of units required for the selected design feed capacity.

All of the other gravity separation models were tested in

a like manner. The results of the testing procedure revealed problem items with each unit operation model, after which they were corrected. As such, the coarse coal jig model was delivered to AspenTech via modem on August 17. The other three models needed to be corrected prior to transmittal, and delivery was completed for the HMV, HMC and table models in September.

Two main items remain unresolved within the gravity separation models:

- 1) For sharp separations (low dp and low Ep values, particularly in heavy-medium vessels and heavy-medium cyclones) the spline interpolation routine does not give an accurate estimate of Ep for the composite partition numbers, and
- 2) The passing of uncleaned fine fractions of coal (misplaced material) through a gravity separation model must be addressed.

These last two items are slated for discussion with project consultant, Dr. Peter Luckie.

CQ Inc. began analysis of data by model discrimination for the form of equation used to describe the partition curve for the heavy-media vessel, heavy-media cyclone, coarse coal jig and concentrating table. Eight equations (logistic, log-logistic, normal, log-normal, Erasmus, Rosin-Rammler, Trawinski, and Lynch) are being evaluated for use in the gravity separation models. The results of the analysis will be documented in the October monthly report.

During the third month of the quarter, relationships between Ep and dp versus particle size were under development for the water-only cyclone, fine coal jig and concentrating spiral. Water balance and equipment sizing algorithms are complete for each device. Model delivery to AspenTech are slated for October and will complete the suite of models required under the category of gravity separation.

3.2.3 Implementing ASPEN PLUS models

The four gravity separation models, coarse coal jig (JIG1), heavy media vessel (HMV1), concentrating table (TAB1), and heavy media cyclone (HMC1), have been implemented and tested as full ASPEN PLUS system models. These models run under the ASPEN PLUS simulator, even in a flowsheet mode having multiple blocks. Washability of product and refuse streams is reported in the block

reports. Design of the format of stream summaries has not yet been completed.

Two new coals were added to the Coal Property Databank. These were a coarse and an intermediate sized coal needed for testing the coarse coal jig and the heavy media vessel models. They will only be used for testing models.

Costing models for the above four gravity separation models have been implemented in ASPEN PLUS. For this a sizing routine and a costing routine have been written for each model. These have been implemented as "USER2" cost models. This poses no limitations for the present, but these models will be converted to system cost models in the near future.

Having implemented the four blocks, they can also be executed with other features of ASPEN PLUS such as a design specifications where the user can find the input D_p that will give a desired ash rejection. An example of this has been run and is reported in Table 1. at the end of this report. The Table 1. shows the full input language but only excerpts of the report in order to make it more concise. This work was actually done in October, 1990, but is so significant that it should be reported now as well as next month.

3.2.4 Dewatering Models

Mechanical Degradation. The existing DOE CoalPrep Simulator uses correlations developed for old-style mechanical centrifuges that contain scrapers and rotating baskets that causes significant amounts of mechanical degradation. Designs developed and used for the past twenty years use vibrating baskets and the degradation is minor. Manufacturers are being contacted to verify the amount of degradation that they use in design.

Solids Loss to Effluent. Manufacturers are also being contacted to verify the amount and nature of the solid that report to the effluent in basket centrifuges. Data is currently being evaluated using CQ Inc. test results from a screen bowl centrifuge and vacuum filter for calculation of classification curves for these devices. It appears that the cut size for vacuum filters is very low (< 37 microns) and indicates 100 percent recovery to filter cake to be appropriate for this model.

Moisture Content. Dr. Richard Hogg provided equations for calculation of the effective mean particle size and

capillary number using modifications to equations used in the models of the existing DOE CoalPrep Simulator. The existing simulator uses weight fraction and only sums over size intervals. These new equations use a volume fraction, more correct for dewatering, and use the geometric mean particle size, an important correction for the finest size interval. Both size and gravity intervals are used in these equations, which will allow differences in coal quality (clean coal versus refuse) to be recognized. In addition, the capillary number equation will contain a term for contact angle, which is related to the hydrophobicity or water-repelling nature of coal. This will also give changes in the moisture content for clean coal versus refuse.

Sensitivity Analysis of DOE Coal Prep Simulator Dewatering Models. Results from this sensitivity analysis show that the existing models do not account for the difference in clean coal and refuse correctly, nor do they account for the amount of fines in the proper manner. Moisture contents obtained for several of the devices by the models were lower than those for operating data. For example, moisture contents for vacuum filters are typically 20-25%, but the model predicts values less than 15%. The corrections that Dr. Hogg has provided should address these issues.

Thermal Dryer. Two possible approaches may be taken for the thermal dryer model. One is the approach in the existing DOE CoalPrep Simulator, which includes a calculation of heat of combustion of coal and tempering of the combustion gases with air to a desired dryer temperature. The second option simply calculates the total heat requirement to evaporate the required amount of water, calculates the air volumes required to carry heat, and then determines the amount of coal needed to heat the dryer air using the Btu content of the coal.

After review, the approach incorporating heat loss calculations and calculations for air and fuel requirements was selected. Coding of the model was completed in September. The model is currently being tested for completeness and accuracy.

3.2.5 Froth Flotation

Evaluation of rate models continued within the work period. Progress has been made in finding data to support development of equations to describe the change in flotation rate and recovery constants due to changes in reagents, solids content and coal rank. The amount of data is limited, however, and several gaps exist. The

forms of many of the equations and the logic for the overall model can be developed based on this data, but additional information should be obtained.

3.2.6 Miscellaneous Items

At the request of DOE, the following information was provided in response to their question concerning data gaps in Task 2:

- (1) Froth Flotation- a systematic study to determine the effect of operating conditions and coal variables on kinetic rate and recovery constants.
- (2) Comminution- a systematic study to determine the effect of coal rank on characteristic crushing parameters.
- (3) Liberation- further quantify the liberation characteristics of coals crushed to different sizes.

During the work period, Dr. L. G. Austin requested several items to enable him to systematically study the comminution and liberation models required for the project. EPRI's Coal Quality Information Book has been provided as a source of information concerning the quantification of liberation occurring during size reduction. Stand-alone models of the roll crushing and rotary breaker processes from the DOE Simulator have been requested as a starting point for his consultations. These models in the previous simulator were developed by Luckie and Austin of Penn State.

On August 13-14 a review of the sizing and costing models was made with Mr. Bill Halvorsen, a consultant to AspenTech, as an independent check of the EPRI Costing Methodology (CCCM). In general, good agreement in methodology was found. Three categories were found to need further verification: (1) pumps appear to be low in cost by about 9 percent; (2) double roll crushers are about one-third the costs quoted by McNally-Pittsburgh; and (3) costs on two-stage crushers appear low by about 30 percent. Mr. Halvorsen has provided additional data for moisture content of centrifuges and comments on our planned output report format for the simulator.


```

30 COMPONENTS H2O H2O / COAL
31 ;
32 DEF-STREAMS MIXNC ALL
33 ;
34 WASHABILITY COAL
35 IN-UNITS SI
36 RETRIEVE FINE-COAL-NO-1 9.52
37 *****
38 ;
39 STREAM DATA
40 ;
41 *****
42 ;
43 SPECIFY INLET STREAM CONDITIONS
44 ;
45 STREAM FEED
46 SUBSTREAM MIXED TEMP=70. PRES=14.7
47 MOLE-FLOW H2O 106.9
48 SUBSTREAM NC TEMP=70. PRES=14.7
49 MASS-FLOW COAL 400.0
50 STREAM MAKEUP
51 SUBSTREAM MIXED TEMP=70. PRES=14.7
52 MOLE-FLOW H2O 0.0
53 SUBSTREAM NC TEMP=70. PRES=14.7
54 MASS-FLOW COAL 0.0
55 *****
56 ;
57 FLOWSHEET DATA
58 ;
59 *****
60 ;
61 FLOWSHEET
62 BLOCK CYC IN=FEED MAKEUP &
63 OUT=PRODUCT REFUSE
64 *****
65 ;
66 BLOCK DATA
67 ;
68 *****
69 ;
70 BLOCK CYC HMC1
71 DESCRIPTION 'PETC HMC1 MODEL'
72 PARAM DP=.5 ; <--- DP = PARTITION DENSITY
73 *****
74 ;
75 *****
76 + U.S. DEPARTMENT OF ENERGY / PITTSBURGH ENERGY TECHNOLOGY CENTER +
77 + ASPEN PLUS COAL CLEANING SIMULATOR +
78 *****
79 ;
80 ;
81 CBLOCK CB1 USER2
82 REFERENCE BLOCK=CYC
83 SUBROUTINE SIZING=SHMC COSTING=CHMC
84 REFERENCE-DATA NUMBER=2 CODES=LENGTH LIQ-FLOW
85 SIZE-RESULTS NRESULTS=1 CODES=DIA
86 ;
87 DESIGN-SPEC TEST
88 DEFINE R BLOCK-VAR BLOCK=CYC SENTENCE=RESULTS VARIABLE=R-ASH
89 SPEC R TO .71
90 TOL-SPEC 1D-1
91 VARY BLOCK-VAR BLOCK=CYC SENTENCE=PARAM VARIABLE=DP
92 LIMITS 1.33 1.77

```

CONVERGENCE STATUS SUMMARY

DESIGN-SPEC SUMMARY

=====

DESIGN SPEC	ERROR	TOLERANCE	ERR/TOL	VARIABLE	CONV STAT BLOCK
TEST	-0.12351E-01	0.10000	-0.12351	1.3300	# LB \$OLVER01

= CONVERGED
 * = NOT CONVERGED
 LB = AT LOWER BOUNDS
 UB = AT UPPER BOUNDS

DESIGN-SPEC: TEST

SAMPLED VARIABLES:

R : SENTENCE=RESULTS VARIABLE=R-ASH IN UOS BLOCK CYC

SPECIFICATION:

MAKE R APPROACH 0.71000
 WITHIN 0.100000

MANIPULATED VARIABLES:

VARY : SENTENCE=PARAM VARIABLE=DP IN UOS BLOCK CYC
 LOWER LIMIT = 1.33000 KG/CUM
 UPPER LIMIT = 1.77000 KG/CUM
 FINAL VALUE = 1.33000 KG/CUM

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
H2O	5712.27	5712.27	0.000000E+00
SUBTOTAL(KMOL/SEC)	5712.27	5712.27	0.000000E+00
(KG/SEC)	102821.	102821.	0.000000E+00
NON-CONVENTIONAL COMPONENTS (KG/SEC)			
COAL	100.798	100.798	0.000000E+00
SUBTOTAL(KG/SEC)	100.798	100.798	0.000000E+00
TOTAL BALANCE			
MASS(KG/SEC)	102922.	102922.	0.000000E+00
ENTHALPY(WATT)	0.000000E+00	0.000000E+00	0.000000E+00

BLOCK: CYC MODEL: HMC1

SOLIDS BALANCE

FEED	=	400.00 TPH
CLEAN COAL	=	185.51 TPH
REFUSE	=	214.49 TPH

WATER / MEDIA BALANCE

	WATER (GPM)	MAGNETIT. (GPM)	MEDIA (GPM)
FEED	= 106.90		106.90
CLEAN COAL	= 3427.36	497.33	3725.76
REFUSE	= 2284.91	198.93	2483.84
CIRC MEDIA	= 5605.37	497.33	6102.70

HMC WATER	=	0.74E+04 GPM
MAKEUP WATER	=	0.56E+04 GPM

EQUIPMENT SIZING RESULTS

HMC SIZE = 20.00 FT
 NO OF UNITS= 6

COST BLOCK SECTION

BLOCK: CB1 MODEL: USER2

*** INPUT DATA ***

PEAK CAPACITY ALLOWANCE FACTOR 1.06

*** FLOWSHEET REFERENCE DATA ***

BLOCK IDENTIFICATION: CYC
 LIQUID FLOW 7409.6029 CUM/SEC

*** SIZING AND COSTING RESULTS ***

CALCULATED NUMBER OF EQUIPMENT 6
 CALCULATED DIAMETER 20.0000 IN

*** COST RESULTS ***

		PER PIECE		TOTAL
CARBON STEEL COST	\$	80,600	\$	483,600
PURCHASED COST	\$	80,600	\$	483,600

END

DATE FILMED

12 / 11 / 90