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INSTRUMENTATION AND PROCESS CONTROL DEVELOPMENT
FOR IN SITU COAL GASIFICATION
QUARTERLY REPORT: DECEMBER 1979 THROUGH
MARCH 1980

MASTER

R. E. GLASS, EDITOR

Prepared by Sandia Laboratories, Albuquerque, New Mexico 87185
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INSTRUMENTATION AND PROCESS CONTROL DEVELOPMENT FOR
IN SITU COAL GASIFICATION

Quarterly Report: December 1979 through March 1980

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Abstract

The analysis of data for the Hanna IV and Hoe Creek in situ coal gasification tests raised questions concerning the fundamental controlling mechanisms of the process. The two main areas of concern are (1) the air flow patterns and (2) the initial cavity growth. Sandia National Laboratories is addressing these concerns by developing models of these processes. Results to date are in qualitative agreement with known phenomena.

There have also been developments in data handling capability. These include improved data presentation ability and development of routine storage, access and back up methods.

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Previous Quarterly Reports for this program are:

Instrumentation and Process Control Development for In Situ Coal Gasification: First Quarterly Report, December 1974 through February 1975, Sandia Laboratories Report, SAND75-0200, April 1975.

Second Quarterly Report, March through May 1975, Sandia Laboratories Report, SAND75-0366, June 1975.

Third Quarterly Report, June through August 1975, Sandia Laboratories Report, SAND75-0353, October 1975.

Fourth Quarterly Report, September through November 1975, Sandia Laboratories Report, SAND75-0669, January 1976.

Fifth Quarterly Report, December 1975 through February 1976, Sandia Laboratories Report, SAND76-0191, April 1976.

Sixth Quarterly Report, March through May 1976, Sandia Laboratories Report, SAND-76-0362, July 1976.

Seventh Quarterly Report, June through August 1976, Sandia Laboratories Report, SAND76-0612, October 1976.

Eighth Quarterly Report, September through November 1976, Sandia Laboratories Report, SAND77-0251, February 1977.

Ninth Quarterly Report, December 1976 through February 1977, Sandia Laboratories Report, SAND77-0669, April 1977.

Tenth and Eleventh Quarterly Reports, March through August 1977, Sandia Laboratories Report, SAND77-1821, December 1977.

Twelfth Quarterly Report, September through November 1977, Sandia Laboratories Report, SAND78-0253, April 1978.

Thirteenth Quarterly Report, December 1977 through February 1978, Sandia Laboratories Report, SAND78-1224, June 1978.

Fourteenth and Fifteenth Quarterly Reports, March through August 1978, Sandia Laboratories Report, SAND78-2311, December 1978.

Sixteenth Quarterly Report, September through November 1978, Sandia Laboratories Report, SAND79-0706, April 1979.

Seventeenth, Eighteenth and Nineteenth Quarterly Reports, December 1978 through August 1979, Sandia Laboratories Report, SAND79-2386, February 1980.

Twentieth Quarterly Report, September through November 1979, Sandia National Laboratories Report, SAND80-0482.

I. INTRODUCTION AND SUMMARY

This report covers the twenty-first quarter of Sandia National Laboratories program on Instrumentation and Process Control Development for In Situ Coal Gasification. This report summarizes program activities conducted between December 1, 1979, and March 31, 1980, in support of the DOE Underground Coal Gasification Program.

The successful development of any in situ fossil energy technology will require a thorough understanding of the chemical and physical mechanisms of the in situ process and its relation to resource geology. The lack of this technical understanding has been a major impediment to development of the positive process control necessary to the efficient utilization of the resource. The Sandia program for Instrumentation and Process Control Development directly addresses this factor.

The overall objectives of the program are: (1) to evaluate instrumentation techniques as they apply to in situ coal gasification, (2) to obtain diagnostic information on the chemical and physical mechanisms associated with this remote process in order to further its understanding, (3) to develop and evaluate remote monitoring techniques and establish their correlation with the process, (4) to develop analytical models for the purpose of process identification, instrumentation development and design, and process modeling, and (5) to develop a process control system utilizing remote monitoring techniques to maximize the recovery of energy by in situ coal gasification. Activities during this quarter contributing to these objectives will be described in this report.

Analysis of the Hanna IV-B thermal data raised questions concerning the fundamental controlling mechanisms in in situ coal gasification. Two of the concerns center on (1) the behavior of the reservoir with respect to varying permeability zones and (2) mechanisms of initial cavity growth during forward gasification. In an attempt to deal with these concerns, two specific areas of interest are being pursued at Sandia. These are (1) a reservoir model with variable permeability and (2) a structural model of the coal seam using the finite element program ADINA. While these models remain in the development stage, initial results indicate that the approaches being used will yield useful results when completed.

In addition to the modeling efforts, this quarter has seen the development and implementation of improved data handling capability. Included

are superior data presentation ability and routine data storage, access and back up methods.

The above accomplishments, while developed with the in situ coal process in mind, are also applicable to all in situ processes. As such, results from this program should have direct application to the development of in situ combustion recovery techniques for other fossil energy resources such as oil shale, tar sands, and petroleum.

II. Modeling

(R. E. Glass, 4737)

A. Reservoir Model

Introduction

During the Hanna IV-B in situ coal gasification test conducted by the Laramie Energy Technology Center (LETC), the linking and subsequent forward gasification occurred in the upper ten feet of a thirty foot seam, resulting in poor resource utilization. The coal seam was ignited in the lower ten feet on April 20, 1979, (Day 110). Shown in Figure 1 is a plot of the temperatures seen during and immediately following ignition. This plot shows temperatures well above the ignition point for coal occurring at the base of the coal seam (0 ft). Also shown are the temperature inside the well casing at the 14 ft level and the calculated temperature that the coal cement interface would see given the known temperatures in the casing. From these data and calculations it is well established that the coal had been ignited at the base of the seam with some small probability of ignition as high as 14 ft into the seam.

Subsequent to ignition, temperatures were recorded in instrument wells throughout this seam. Three days after ignition the first thermal response was detected in a well approximately 15 ft from the ignition well (Well BB) at an elevation of 9 ft indicating that the linking process was progressing as expected. The following day, however, saw the same well recording a response at the 25 ft level with no intermediate response. Figure 2 gives the temperature profiles for Well BB clearly showing the two separate paths. This indicates the presence of two distinct flow paths. Subsequent responses during both reverse combustion and forward gasification lay primarily in the 20 to 30 ft region.

Figure 1. Temperatures at the ignition well.

Figure 2. Thermocouple response in Well BB showing the approach of two separate linkage paths.

Examination of well logs, shown in Figure 3, done prior to the test shows high permeability zones in the 20-30 ft region.

The result of ignition low in the seam followed by thermal responses high in the coal seam near previously established high permeability zones lead to the questioning of the effect of high permeability zones both natural and man made. It was decided this question could best be investigated by developing a reservoir model.

Figure 3. Well logging demonstrating high permeability regions between 20 and 30 ft. (After Bartel¹)

The Model

The model presently being developed is for two phase flow through a porous media. The governing equations for the model are

$$\nabla \cdot \left[\frac{kT\rho_w k_{rw}}{\mu_w} (\nabla P_w + \rho_w g \Delta h) \right] + Q_w = \phi T \frac{\partial}{\partial t} (\rho_w S_w) \quad (1)$$

and

$$\nabla \cdot \left[\frac{kT\rho_n k_{rn}}{\mu_n} (\nabla P_n + \rho_n g \Delta h) \right] + Q_n = \phi T \frac{\partial}{\partial t} (\rho_n S_n) \quad (2)$$

where

- k = permeability
- T = seam thickness
- ρ = density
- μ = viscosity
- P = pressure
- g = gravitational constant
- h = height
- t = time
- S = saturation
- Q = injection rate

subscripts

- r = relative
- w = wetting phase
- n = nonwetting phase

The injection rate, Q_t , is specified. The production rate is given by

$$Q_n = Q_t \lambda_n / (\lambda_n + \lambda_w) \quad (3)$$

$$Q_w = Q_t - Q_n \quad (4)$$

where

- Q = volumetric flow rate
- λ = mobility

The model was initially patterned after the Blair and Weinaug² fully implicit model, but was later modified using Peaceman's³ semi-implicit saturation.

$$S' = \frac{S_{n_{i,j,m+1}} - S_{n_{i,j,m}}}{P_{c_{i,j,m+1}} - P_{c_{i,j,m}}} \quad (5)$$

where

S' = time rate of change of saturation

P_c = capillary pressure

and the subscripts

i = horizontal mode

j = vertical mode

m = time step.

This modification eliminated some problems with negative capillary pressures resulting from poor initial estimates for flow rates and pressures. An additional piece of information necessary to solving the equations is the saturation relationship,

$$S_n + S_w = 1 \quad (6)$$

The governing equations having been selected, it becomes necessary to have four boundary and one initial condition for each of equations (1) and (2). This is achieved by assuming (1) an initial pressure distribution for each phase and (2) impermeable boundaries. The first assumption yields

$$P_1(x,y,0) = P_0(x,y) \quad (7)$$

and the second assumption yields

$$\frac{dP_i}{dx} \quad y = 0, l_1 = 0 \quad (8)$$

$$\frac{dP_i}{dy} \quad x = 0, l_2 = 0 \quad (9)$$

where the reservoir is bounded by the sides $x = 0$, $x = l_2$, $y = 0$, $y = l_1$, and the subscript i denotes either the wetting or the nonwetting phase.

Since the relative permeabilities are functions of the saturation, which is a function of the capillary pressure, it is necessary to obtain either a functional or tabular form for these. These were given in Taber *et al.*⁴ and Fulton and Reznik⁵. This data is summarized in Figures 4 and 5.

The governing equations were written in finite difference form and solved using successive overrelaxation. Figure 6 shows the kind of results available. The program was run with an injection rate of 10^{-2} kg/s at 10^6 N/m² pressure. While qualitative phenomena such as buoyancy are predicted, there remain problems with overall material balances.

Possible modifications to the program include (1) use of a semi-implicit production term or (2) use of pressure conditions at the injection and production wells instead of flow rates.

Figure 4. Capillary Pressure, P_C , vs. Water Saturation, S_w for Pittsburgh Coal (After Taber)

Figure 5. Relative Permeabilities as a Function of Water Saturation (After Fulton and Reznik⁵)

Figure 6. Air Saturation as a Function of Time at the Injection Block.

An alternative approach to the problem is to write equations (1) and (2) as a set of first order ordinary differential equations of the form

$$dS_1/dt = f_1(x, \lambda),$$

$$dS_2/dt = f_2(x, \lambda),$$

.

.

.

$$dS_n/dt = f_n(x, \lambda).$$

and solve these in an iterative loop with the aid of one of Sandia's in-house codes.⁶ This approach has been programmed but has not yet produced useful results.

B. Structural Model

Introduction

Another area of concern in the development of the in situ coal gasification technology is the initial cavity growth. There are numerous factors affecting the initial cavity including heat and mass transfer, chemical kinetics and mechanical stress and failure. Extensive work in the areas of heat and mass transfer and chemical kinetics has been done by such authors as Edgar et al⁷ and Schwartz et al.⁸ There has also been work in mechanical stress especially in relation to subsidence effects by Advani et al.⁹ and Greenslaw et al.¹⁰ The present model is being developed to look more closely at the area immediately surrounding the cavity to determine the stresses and probable failure zones.

The decision to concentrate on mechanical properties arises from the shape of the cavities formed at Hoe Creek II, Hoe Creek III, and Hanna IV. An example of the cavities formed is given by Hill and Minkel¹¹ in a discussion of the postburn coring program for Hoe Creek II. These results in conjunction with the override problems seen at Hoe Creek III and the two Hanna IV experiments indicate that the initial vertical growth of the cavity is a determining factor in the in situ process. The present modeling activity is aimed at determining if mechanical failure is sufficient to explain the phenomena provided all other mechanisms act isotropically.

The Model

Since the problem of interest is one of structural analysis, it was decided to use the previously developed finite element program ADINA.¹² The nodal points for the input to ADINA were generated using QMESH.¹³ The mechanical properties of coal were from Advani *et al.*⁹

Results

The model was run with one time step to determine the effects of the lithostatic pressure acting on a coal seam with a small rectangular cavern. The lithostatic pressure was assumed to be 10 atm, the cavern was assumed to be one foot high by two feet across in a coal seam 30 feet high and 200 feet across. Shown in Figure 7a is the undeformed mesh generated by QMESH for the 10 ft by 10 ft area around the cavern. The view is a cross section of the coal seam looking down the hole. The program assumes the seam is axisymmetric about the Z-axis. The R-axis represents the seam floor and is allowed only horizontal displacements while the Z-axis is allowed only vertical displacement. Figure 7b shows how the coal deforms when lithostatic pressure is applied to the top of the coal seam ($Z = 30$) and gravity is acting throughout the seam. The deformations in Figure 7b are magnified by a factor of 380.

While the deformations allow the process to be visualized, the matter of most concern is the stress distribution. The maximum stress (least compressive) contours are shown in Figure 8. The model also produces various other stresses, however, since coal fractures more easily under tensile stresses,¹⁴ these are of greatest interest. The stress contours shown in the figure are all compressive. The tensile stresses were noted in the detailed printout to occur only in the area near the center of the roof of the cavern. This is encouraging since failure there would lead to the vertical growth of the type seen at Hoe Creek II and as predicted in roof subsidence studies.

Future Modifications

Since work on the stress and failure patterns has just begun, there are many additions to be made. These include incorporating temperature distribution effects and different initial cavity shapes. The temperature patterns can be generated by ADINAT¹⁵ and different mesh shaped caverns can be generated by QMESH.

Figure 7. The coal seam (a) before and (b) after lithostatic and gravitational forces act. Deformations in (b) are magnified by a factor of 380.

Figure 8. Maximum stresses (least compressive) induced in a coal seam with lithostatic pressure and gravity. (Cavern Crosshatched)

III. DATA SYSTEMS

A. Plotting Routines

(P. C. Kaestner, 4737)

The large amount of data being received and processed from field experiments has necessitated the development of software capable of presenting the data in a coherent and readily available form. The magnitude of the problem is apparent when it is realized that the thermocouple data from Hanna IV-B alone consists of over 3.5 million words. The quantity of data in conjunction with time constraints imposed by the user requires that efficient means be developed for reading and presenting the data. The plotting developed to accomplish these objectives will be described in the following paragraphs.

Software

The plotting programs have as a common building block the Dicomed-Zeta plotting package. The Zeta plotting package interfaces with the Fortan program and gives the programmer access to the plotting capabilities of the Zeta plotter (an X-Y incremental pen plotter), or the terminal screen (an HP 2648A). The Dicomed plotting package interfaces with the Zeta package as if it were another device in the Zeta package. The Dicomed package gives the programmer access to all of the film graphic capabilities of the Sandia Central Computing Facilities. These include movies, both 16 and 35 mm, in color or black and white and microfiche at both 24 and 48X. This access is via magnetic tape written by the lab system and used on the Dicomed. The tape, once written, may be processed in any of the available modes.

Using the Dicomed-Zeta plotting package as a base, several plotting routines were developed to present the various types of data with options as to the media of production. The remainder of this section will describe the individual routines.

PLOTWELL generates a plan view of the well pattern at the Hanna IV site. It can be easily modified to other locations. The primary output medium is the terminal screen, but output on the Zeta plotter is possible. The program itself is short and fast, operating with a minimum of user interaction. Variants of this program are used to study Hanna IV-A or Hanna IV-B, or subsets of the entire well pattern.

PLOTFICHE generates a time versus temperature history of a given measurand. The time interval is specified by the user and may be as large as 200 days. The temperature axis limits may be picked by the user or generated by the program. The measurand is either specified by the user or is a measurand in the user chosen well. The output media include the terminal screen, the Zeta plotter, or via magnetic tape to the Dicomed plotter and on to microfiche. The user interaction is reasonable considering the number of options available. The program is large. A number of techniques are used to speed up the data acquisition process, but the number of numbers involved still cause the program to seem slow. The average well has 12 or 16 measurands, and core limitations dictated that no more than four measurands could be held at any one time. This forced three or four passes over the same records to retrieve all data for a given well. The new memory available for the system will ease the problem.

The program currently works on the Hanna or Rock Springs sites and with some modification will work on other sites.

TVSD generates a temperature versus depth graph for a given well. The program determines all measurands in a well, and their temperature at a given time. It orders the measurands from shallow to deep and generates the plot. User inputs are minimal. The program is not large. Once the measurands in the well are determined, the program will pick up new times quickly.

GKON generates plan view temperature contours at a given level over a time period. The programs output medium is color film, though the user can chose any other available device. User interaction with this large program is minimal. The set of measurands which define the level are a part of the program. While the technique can be used on any site, this program is site specific, tied by such things as the measurands and the titles.

A general technique for taking a few data points in a field and generating regularly spaced data on the field was developed. The technique involves finding the N ($2 \leq N \leq 5$) nearest neighbors to the point at which the temperature is desired. The temperature at the point is a reciprocal distance weighted average of these neighbors modified by their angular separation viewed from the desired point. Neighbors separated by less than 90 degrees have their weighting factor reduced by the sine of the angle.

The contouring subprograms are an improvement over the contour package described by Milly¹⁶. GKON's speed is reasonable considering the number of options and calculations. A four-minute movie in color takes about two hours of computer time, and covers about eight days of burn.

B. Data Base Management (D. L. Brown, 4737)

The growth of the data base acquired from in situ coal gasification tests has been such that improved data base management software was needed. The following paragraphs summarize the programs developed for this purpose.

The program, FMSRTP, produces a sorted and compacted file management report with summary information to manage the disk files and disk space

allocation. The input data is the file name, initial size, maximum size, and volume name. A tree sort is employed and the report is produced for a print output device. Special features include compactness, number of files cataloged, and number of tracks allocated for these files. There is a stored procedure that executes the program to produce the report on demand.

A redundancy routine has been incorporated in a program that transfers the data from field experiments to the laboratory computer disk storage. This routine recalculates the disk pointers, positions the magnetic tape and continues to store data. Prior to incorporating this routine, it was necessary to wait until a replacement tape was recreated and to reload all the data that had been previously stored.

In addition to the software improvements, two new components have been added to the hardware. These include floppy disks and a memory expander. The floppy disks are being used to provide back up and recovery capability for programmer libraries and some of the data. The memory expander doubles the memory capacity from 128 kbytes to 256 kbytes. This additional memory allows several programs to run on the system simultaneously without serious degradation of efficiency.

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PUBLICATIONS, PRESENTATIONS, AND OTHER COMMUNICATIONS

A. Publications

1. R. E. Glass (Editor) "Instrumentation and Process Control Development for In Situ Coal Gasification: Twentieth Quarterly Report, September through November 1979, "Sandia Laboratories Report SAND80-0482.

B. Presentations

1. T. L. Dobecki and L. C. Bartel presented a paper entitled "Geophysical Site Characterization for Underground Coal Gasification in Washington" at the Northwest Mining Association's 85th Annual Convention, Spokane, WA, December 6-8, 1979.

C. Other Communications

1. B. E. Bader and P. J. Hommert attended the Coal Management Team meeting in Germantown, MD, December 18-20, 1979.
2. L. C. Bartel attended LLL's briefing on the Hoe Creek III experiment in Livermore, CA, on January 23, 1980.
3. L. C. Bartel and S. L. Love gave a briefing on the status of the Washington State program to the State of Washington Governor's Task Group on Alternate Energy Sources in Olympia, WA, on January 29, 1980.
4. P. J. Hommert gave a briefing on Sandia's UCG activities to EXXON personnel on February 6, 1980, in Albuquerque, NM.
5. L. C. Bartel worked at DOE Headquarters in Germantown, MD, from February 13 to February 22, 1980.
6. B. E. Bader attended a UCG management meeting at the San Francisco office in Oakland, CA, on February 19, 1980.
7. R. E. Glass attended a seminar on flow through porous media of the University of New Mexico in Albuquerque, NM, on February 25, 1980.

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