THE UNIVERSITY OF ALABAMA
COLLEGE OF ENGINEERING
BUREAU OF ENGINEERING RESEARCH **MASTER**

QUARTERLY REPORT

on

ARC Contract No. 77-121-AL-5605-77-IR-302-0830

and

DOE Contract No. DE-AS05-78ET10182

FEASIBILITY STUDIES OF IN-SITU COAL GASIFICATION
IN THE WARRIOR COAL FIELD

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Prepared for

The Appalachian Regional Commission
Washington, D.C. 20550

and

The Department of Energy

January 1980

BER Report No. 252-124

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Quarterly Report to
The Department of Energy
and
The Appalachian Regional Commission

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The University of Alabama

January 1980

FORWARD COMBUSTION IN CHAR

Mark Griffin

During this report period experiments were completed with the tube furnace combustor described previously. As of early December, a total of 47 burns had been made using char produced from coal from Alabama's Blue Creek seam. Of these, 35 runs produced usable results. With the completion of the experimental program, a large data base is now available from which the combustion characteristics of the char can be determined.

The burn program involved independent variation of three parameters: initial fuel bed temperature, applied air flow, and water vapor influx rate. Three furnace settings were applied, these being 1000, 1400, and 1800 degrees F. Four flow rates were studied ranging from near zero to a maximum of 3.5 standard liters per minute. Water vapor was varied so as to yield hydrogen/oxygen ratios of 0., 0.5, and 1.0 in the fuel bed.

Following completion of the experiments, temperature and gas analysis data were reduced to determine fuel bed temperature profiles and off-gas quality as functions of time. Temperatures in the char showed a strong dependence on air flow at the lower temperatures, with a standing thermal wave characteristic of the oxidation-reduction zones traversing the bed in the course of the burns. Thermal profiles at the higher initial temperatures tended to be much more flat. Observed temperature profiles for three cases at the same flowrate are shown in Figures 1-3.

Gas quality from the char bed ranged from poor to good, with the

higher temperatures and H/O ratios yielding carbon monoxide and hydrogen mixtures with heating values in the range of 160 BTU/cu ft. Low temperature burns generally produced little usable gas due to insufficient reduction reaction rates.

Plots of gas quality vs. time for most cases appear as standing waves. This indicates the majority of the combustion reactions take place in a length of the fuel bed less than the total length. This seemed particularly true for burns made without the addition of water vapor. Typical results illustrating the effect of variation of water influx are shown in Figures 4-6.

At this time numerical finite difference models are being written. Using these and the data from experimental burns we intend to generate empirical reaction rates for this particular char as functions of temperature. With these results and other work done by Wong and Mohan (see previous progress reports) predictions of gas quality for arbitrary thermal profiles are possible. We plan to then use thermal conductivity data from Mr. Fong's work on this project to predict limiting conditions for successful in-situ burns.

I. THERMAL CONDUCTIVITY AND THERMAL DIFFUSIVITY OF COKE

Y. R. Fong

INTRODUCTION

Thermal conductivity and thermal diffusivity of coke are some of the important physical properties in combustion. They determine the rate and extent of pyrolysis away from a burning zone and the rate of propagation of the flame front. Calculations of the temperature profile within a porous solid during heating require a knowledge of the numerical values of the thermal conductivity and thermal diffusivity of coke and the variation of these quantities with temperature.

To determine thermal conductivity, a knowledge of the rate of heat flow through a given area of a specimen under a known temperature gradient is necessary. The simplest and most common arrangement for this determination involves flow in only one dimension. The chief difficulties here arise from heat losses and these may be minimized by the use of silica aerogel for insulation and by the employment of guard rings. This means that the heat flow is measured only for a central portion of the area where it is uniform. Radial flow methods eliminate most of these losses but have difficulties of their own. Periodic or other variable state (as regards temperature - time relations) methods have sometimes been used to determine conductivity, but more generally to determine diffusivity.

THEORY

Of the methods for measuring thermal conductivity of solids at

high temperatures, those employing linear and quasi-linear heat flow are the most important group. The Thermophysical Properties Research Center (TPRC) data books list about 800 references pertaining to the measurement of thermal conductivity of solids, of which about 600 employ essentially linear heat flow. These divide about equally into work below and above room temperature, and of the latter, about half date from 1950, the other half having been published during the preceding hundred years.

The methods of measuring thermal conductivity can be classified readily into groups according to the principles of operation that they follow. The selection of the best techniques should be based on an extensive mathematical analysis of the heat-flow problems associated with linear and quasi-linear methods of measuring thermal conductivity. Rather than to give an exhaustive account of methods of conductivity measurement, only several standard methods are discussed here.

Methods of measuring thermal conductivity

- A. Classification according to the mode of heat flow
 - 1. Linear flow method
 - 2. Radial flow method
- B. Classification according to the state of heat transfer
 - 1. Steady state method
 - 2. Dynamic (transient) method

A-1. Linear flow method

One-dimensional flow of heat includes the common cases of flow of heat through a thin plate or along a rod, the two faces of the plate, or ends of the rod, being at constant temperatures T_1 and T_2 . In other words, linear flow occurs when the flow of heat in any body is

such that the isothermal surfaces, or surfaces of equal temperature, are parallel lines. For these cases the general equation of steady state conduction reduces to

$$\frac{d^2T}{dx^2} = 0 \quad 1$$

The standard method ¹⁰ is to sandwich a flat electrically heated element between two similar flat slabs of the material under test, on the farther side of which are water-cooled plates. A guard ring is used to prevent losses that might otherwise be large.

In a method ¹¹ useful for thin materials such as mica, the specimen is clamped between the ends of two copper bars, one of which carries a heating and the other a cooling coil. The heat flow is determined by measuring the temperature gradient along the bar with thermocouples, the conductivity of the copper bars being known. This method has also been developed so that it can be used at various points on a sheet of continuous material.

A-2. Radial flow method

Radial flow occurs when heat flows in more than one dimension, namely of spherical and cylindrical flow. For flow of heat in a sphere, the rectilinear coordinates, x, y and z are replaced by a single variable r. This is done by the following transformation:

$$\frac{\partial T}{\partial x} = \frac{\partial T}{\partial r} \cdot \frac{\partial r}{\partial x} = \frac{\partial T}{\partial r} \cdot \frac{x}{r} \quad 2$$

because, since $r^2 = X^2 + Y^2 + Z^2$

$$\frac{\partial r}{\partial X} = \frac{X}{r}$$

also

$$\frac{\partial^2 T}{\partial X^2} = \frac{d^2 T}{dr^2} \cdot \frac{X^2}{r^2} + \frac{dT}{dr} \cdot \frac{1}{r} - \frac{dT}{dr} \cdot \frac{X^2}{r^3}$$

3

with similar expressions for the derivatives with respect to y and z.

We thus obtain

$$\begin{aligned} \nabla^2 T &= \frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} \\ &= \frac{d^2 T}{dr^2} + \frac{2}{r} \cdot \frac{dT}{dr} \end{aligned}$$

4

since, however,

$$\frac{d(rT)}{dr} = r \frac{dT}{dr} + T \quad \frac{d^2(rT)}{dr^2} = r \frac{d^2 T}{dr^2} + 2 \frac{dT}{dr}$$

we have

$$\nabla^2 T = \frac{1}{r} \cdot \frac{d^2(rT)}{dr^2}$$

5

The Fourier equation for steady radial heat flow becomes

$$\frac{1}{r} \cdot \frac{d^2(rT)}{dr^2} = 0$$

6

When materials, particularly poor conductors, can be formed into cylinders or hollow spheres, the radial flow method may be useful. This has the advantage of largely or even totally eliminating lateral heat losses.

A standard method ¹¹ of measuring the conductivity of some types of insulating material is to wrap the material about an electrically heated cylinder or pipe. The cylinder has an extension or guard ring at each end, and only the heat input into the central section is used in the measurement, thereby eliminating end losses.

B-1. Steady state method

The thermal conductivity is measured with an experimental arrangement which must simulate a solution of the differentiate equation defining the conduction of heat in a homogeneous isotropic solid.

$$\nabla^2 T = \frac{1}{\alpha} \cdot \frac{dT}{dt} \quad 7$$

The general reduction of Equation 7 consists of a term defining the temperature change in steady state and also a transient relating the temperature change with time. The steady state term leads, for unidirectional flow of heat and no radial heat losses, to

$$Q = -K \frac{[T_o \quad T_L]}{\int_0^L \frac{dL}{A}} \quad 8$$

For heat flow in a cylinder between radii r_1 , and r_2 ($r_2 > r_1$) and no longitudinal heat losses Equation 8 may be rewritten as

$$Q = -K \frac{[T_{r_1} \quad T_{r_2}]}{\int_{r_2}^{r_1} \frac{dr}{2\pi r}} \quad 9$$

The steady state solution Equation 8 becomes

$$Q = KA \frac{\Delta T}{L} \quad 10$$

and may be simulated experimentally with little difficulty especially at moderate temperatures. Test apparatus is not standardized universally and variation in the size and shape of the sample occur as does the orientation of the equipment.

B-2. Dynamic method 15,4,6

Dynamic methods simulate the variable state term in the general solution of Equation 7 with appropriate boundary conditions. If a large solid which is initially at a constant temperature suddenly has one surface raised to a higher temperature, the temperature distribution in the body has a function of location and time is given by the solution of the heat conduction equation:

$$\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} = \frac{1}{\alpha} \left(\frac{\partial T}{\partial t} \right) \quad 11$$

where α is the thermal diffusivity.

Some other techniques are normally referred to as line source or probe methods and the basic configurations involve a thin wire or foil embedded in the test material with as good contact as possible. Dynamic technique for measuring thermal conductivity in a cylindrical geometry as in "Hot Wire Method" has the following desirable features:

- i. faster than steady state method (less than 12005 depending upon boundary conditions);

- ii. not restricted to finding k for dry materials;¹
- iii. unlike other dynamic techniques, a precise knowledge of thermal diffusivities or specific heats is not required, and cylindrical specimens are not assumed infinite in the radial dimension;
- iv. thermal conductivities may be calculated from a simple relationship between heat inputs and temperature differences.

Theory of Hot Wire Method

A. Determination of Thermal Conductivity:

The method was developed by E.F.M. van de Held and F.G. van Drunen¹⁷ for determining the thermal conductivity of poor conductors and has been applied in the present case to determine also the thermal diffusivity.¹⁰ This method can be classified to be a dynamic radial flow method.

An electrically energized line heat source is inserted into the medium whose thermal conductivity is required. A line source may be thought of as a continuous series of point sources along an infinite straight line. The flow of heat from a point source in a thin plate sheet or lamina, if there is no radiation or other losses from the sides, may be considered as a special case of line source, perpendicular to the plane, since the heat flow is all normal to such a line source, i.e. radially in the plane. Initially the temperature of the medium is uniform. The heat source is instantaneously turned on and heat is released at a rate of q per unit length. The temperature T at any point in the body will be a function of time t measured from the

¹ Important since thermal conductivity is affected by moisture. This is particularly true for building insulation and soils. It is also important for high temperature use when materials may be chemically or otherwise unstable or contamination may take place when test samples are exposed for long duration to such environments.

moment the current is turned on, the thermal diffusivity α of the material, and the radial distance r measured from the line heat source. The mathematical expression for radial flow of heat in a cylinder is: ^{12,5}

$$\frac{\partial T}{\partial t} = \alpha \left[\frac{\partial T}{\partial r} + \frac{1}{r} \frac{\partial T}{\partial r} \right] \quad 12$$

which has a solution

$$T = \frac{q}{2\pi K} \int_0^t \left[\text{EXP} \left(-\frac{r^2}{4\alpha t} \right) \right] dt \quad 13$$

by using the substitution

$$\beta = \frac{r}{(4\alpha t)^{1/2}} = r\eta \quad 14$$

Equation 13 becomes

$$\begin{aligned} T &= \frac{q}{2\pi K} \int_{r\eta}^{\infty} \frac{e^{-\beta^2}}{\beta} d\beta \\ &= \frac{q}{2\pi K} [I(r\eta)] \end{aligned} \quad 15$$

The thermal conductivity k , and the thermal diffusivity α are assumed constant over the range of temperature occurring within the medium. The exponential integral for small values of $r^2/4\alpha t$ may be approximated by a series expansion:

$$I(r\eta) = \ln\left(\frac{4\alpha t}{r^2}\right) + \frac{1}{2}\left(\frac{r^2}{4\alpha t}\right) - \frac{1}{8}\left(\frac{r^2}{4\alpha t}\right)^2 + \dots - \frac{\gamma}{2}$$

where γ is Euler's constant = 0.5772156

since $(r^2/4\alpha t)$ is small, $I(r\eta)$ can be approximated by

$$I(r\eta) = -0.2886078 + \ln \frac{(4\alpha t)^{1/2}}{r} \quad 16$$

the error in this approximation is less than 5 percent when β is less than 0.3. Substitution of Equation 16 into Equation 15 gives

$$T = \frac{q}{4\pi K} \left[\ln t + \ln \left(\frac{4\alpha}{r^2} \right) - 0.5772156 \right] \quad 17$$

To apply this equation in the hot wire method, we let T_0 be the initial uniform temperature at time t_1 and T_r be the temperature at a radial distance r from the heat source after A time t_2 . Then the rise in temperature at a point in the medium will be given by

$$T_r - T_i = \frac{q}{4\pi K} [I(r\eta)] \quad 18$$

Thus the thermal conductivity can be calculated from the slope of a plot of the temperature rise at a point close to the heat source against the natural logarithm of time which is $q/4\pi k$ irrespective of the distance r provided β is less than 0.3. It is obvious that

a plot of temperature against $\ln t_2$ should be a straight line with the slope $q/4\pi k$. Thus k can be obtained by the knowledge of this slope and the applied power per unit length of the heat source.

B. Determination of Thermal Diffusivity:

To determine the thermal diffusivity the temperature is also observed at another point which is at a greater, measurable distance from the heater wire. A simple rearrangement of Equation 18 gives

$$I(r\eta) = \frac{2\pi K}{q} (T_r - T_i) \quad 19$$

The right-hand side of Equation 19 can be evaluated from the measurements of T_r , T_i and the value of $q/4\pi k$, given by the slope of the logarithmic plot used to determine the thermal conductivity. The values of β corresponding to these values of $I(r\eta)$ given by Equation 18 may be obtained from Tables of $I(r\eta)$.² The thermal diffusivity X is then calculated from β by means of Equation 14 for the known values of r and t .

EXPERIMENT

In order to obtain data on thermal conductivity and thermal diffusivity of coke, the following experimental steps have been taken:

1. Preparation of samples
2. Carbonization of coal samples
3. Measurement of temperature rise resulting from heat supplied

² Values of $I(r\eta)$ is computed and tabulated by L. R. Ingersoll, et al in Heat Conduction: with engineering, geological, and other applications in Appendix F.

by the heater wire.

Stage 1: Preparation of samples.

Coal samples were collected from different coal mining areas in Northern Alabama. The samples were taken from roadcuts and mines along the western side of the Warrior coal field, generally within a few miles either side of Alabama Highways 43 and 13. A proximate analysis was performed on the coal samples according to the ASTM Standard Methods of Laboratory Sampling and Analysis of Coal and Coke (ASTM Designation: D271-48). The coal samples were tabulated according to their moisture content, volatile matter, ash content and fixed carbon respectively. Coals with similar properties were grouped together and a representative was chosen from each group. After much iteration, selection and elimination, eleven samples of coal were chosen to be the representative. They are tabulated in Table I.

Lumps of coal were reduced to about 3.75 inches x 3.75 inches x 5.0 inches with the use of a diamond saw. The corners of each piece were rounded off so as to fit into a cylindrical container. A stainless steel container was designed (see Fig. 1). The perforated plate allows volatile matter and fluid products to pass through while constraining the coal within a fixed volume. Strong material was used to ensure that the coke container could withstand the large expansion in volume during pyrolysis. In order to simulate the conditions of coal carbonization underground, the remaining spaces in the container was filled by a high-temperature refractory called steelkon.³ A small amount of water was added to the refractory and made into a paste form.

³ Steelkon -- is a commercial 2800°F blast furnace castable manufactured by A.P. Green Refractories Co.

TABLE I

PROXIMATE ANALYSIS OF ALABAMA COALS ON THE "AS RECEIVED" BASIS
AND ON THE "MOISTURE FREE" BASIS, NUMBERS
ARE ON WEIGHT PERCENTAGE

As Received		Moisture Free		
Sample Name	Moisture	Volatile Matter	Ash	Fixed Carbon
Utley 1-A	1.3	36.8	9.9	53.3
Utley 1-B	1.5	37.5	7.3	55.2
Pratt 2	1.6	40.5	5.2	54.3
Utley 3	1.5	43.1	4.1	52.8
Upper Cobb 4	2.0	43.8	4.7	51.5
Corona 5	2.6	41.7	4.8	53.5
Thomas 6	2.1	38.5	7.9	53.6
Upper Cobb 7	2.0	38.2	4.8	57.0
Gillespy 8	4.6	40.3	2.7	57.0
Blue Creek 9-A	5.05	30.2	14.8	55.0
Blue Creek 9-B	2.48	31.4	24.2	44.4
Mary Lee 10	1.93	39.6	12.1	48.3
Mary Lee 11	2.37	32.7	10.0	57.3
Jagger 12	1.67	37.5	6.2	56.3
Blue Creek 13	2.59	36.2	12.1	51.7
Pratt 14	2.02	43.1	5.9	51.0
Jefferson 15	3.45	36.6	4.1	59.3
Black Creek 16	3.54	38.5	4.5	57.0
Blue Creek Type A	2.42	35.6	8.1	56.3

Fig. 1. Cylindrical Coke Container

The wet steelkon was stuffed into the remaining spaces between the coal and the container. The refractory was left in air to dry. In this way the coke would be formed under volume constraint similar to the situation underground.

To perform tests to determine thermal conductivity and thermal diffusivity of coke, the thermocouples were embedded in the coke before pyrolysis to ensure proper contact. A 0.1 inch (2.5 mm) diameter hole was drilled centrally through the coal and two other 0.067 inch (1.5 mm) holes were drilled to the midplane of the cylindrical sample parallel to the central hole; one as close as possible and the second one 15 mm away. A 26-gauge chromel A wire was used as a heater wire and was inserted through the central hole. The two thermocouples were inserted into the other two holes respectively. The top and bottom lids were bolted to the flanges of the container which were sealed with asbestos gaskets. A tubing was screwed onto the threaded-hole on the top lid for the escape of volatile matter and tar. All the wires were insulated from coal which becomes electrically conducting at high temperatures, with ceramic insulation sleeves. A 1.5 inch diameter hole was drilled on the door of the electric furnace⁴ for the passage of the exhaust tubing. The hole also provided an outlet for the thermocouples. An extra thermocouple was used to monitor the temperature of the furnace. The thermocouples were connected to a data logger.⁵

⁴ Fisher Isotemp Muffle Furnace Model 186, 1134 cubic inches, (18,567 cc), maximum temperature 1100°C (2012°F), 240 V, 50/60 Hz, Fisher Scientific Company, Atlanta, Georgia.

⁵ Instrulab 200 Data Logger, Instrulab Inc. Dayton, Ohio.

Stage 2: Carbonization of Coal

A vacuum pump was used to evacuate the air and moisture from the coal sample. The furnace was turned on and the sample was heated up in a slow stream of nitrogen to provide an inert atmosphere and thus prevent oxidation of the coal. After the maximum temperature of 850°C has been reached, the sample was allowed to pyrolyze for two more hours before cooling.

Stage 3: Determination of Thermal Conductivity by Hot Wire Method

After the furnace had cooled down, the exhaust tubing was removed. One end of the heater wire could be retrieved through the threaded-hole. The two ends of the heater wire were connected to the DC power supply. The coke was placed in the electric furnace and heated in a slow stream of nitrogen to the temperature at which a test was to be made. Before each test, the heating rate was reduced to less than 0.5°C per minute and the rate of rise of temperature of the lump was measured over a period of 20 minutes. The current for the heater wire was supplied by the DC power supply. Temperature/time readings of the thermocouples were recorded by the data logger (see Fig. 2). The first set of readings was taken at room temperature. New sets of readings were recorded at every increment of 50°C (approximately) until up to 900°C. Hence a total of 18 sets of readings were taken. Heat was supplied at a constant rate until the desired temperature had reached. Then the thermostat turned the heaters on and off in order to maintain the temperature. Measurements of the thermal conductivity were commenced when the rate of rise of temperature was less than + 0.1°C per minute. The thermal conductivity was calculated from the slope of the plot of the corrected temperatures of the point close to the heater wire

Fig. 2. Schematic for Hot Wire Method

against $\ln t$ which by Equation 17 is equal to $q/4\pi k$. The thermal diffusivity was calculated from Equation 14, as described earlier, at various times from the start of the test. The mean of these values of α was taken as the thermal diffusivity corresponding to the initial temperature of the test. The furnace was then raised to a higher temperature and the tests repeated.

DISCUSSION

Several more runs had been made since the last quarterly report. The experiment was slowed down due to the burning up of electrical wire during the hot wire method experiment. After the coke was made, copper electrical wires were connected to the two ends of the Nichrome wire embedded in the coal before pyrolysis. The Nichrome wire was being used as the heating source in the hot wire method testing. Although the electrical wires were protected by ceramic insulation sleeveings, they cannot stand high temperatures. As a result, different kinds of copper electrical wire and steel wire of different gage sizes and different types of ceramic insulations had been tried. All of them did not show satisfactory results. Finally, it was discovered that using Nichrome wire of large gage size is the best alternative. The two pieces of Nichrome wire connect the two ends of the Nichrome heating wire, which was embedded in the coke, and extend to the outside of the furnace where another section of ordinary electrical wire connects them to the D.C. power supply. The Nichrome wire proved to be able to stand high temperature and yet will not increase the temperature inside the furnace which is at a steady state temperature.

Two successful runs have been completed on Thomas Coke (sample No. 6) and Mary Lee coke (sample No. 11). Plots of thermal conductivity and thermal diffusivity vs temperature of the samples are attached (Figs. 3,4,5,6). An overall conclusion will be drawn upon completion of tests on all samples.

THOMAS COKE

SAMPLE NO. 6

Temperature (°C)	Thermal Conductivity (WATT/m°C)	Thermal Diffusivity (cm ² /sec)
100	0.6754	0.001618
172	0.8920	0.0030217
177	0.7847	0.003697
235	0.89959	0.00400
300	0.9464	0.004283
388	1.3252	0.005167
426	1.4821	0.007876
495	1.5193	0.006571
521	1.1983	0.007824
596	1.554	0.00976
642	1.5182	0.00832
662	2.226	0.00867
730	2.295	0.01184

MARY LEE COKE

SAMPLE NO. 11

Temperature (°C)	Thermal Conductivity (WATT/m°C)	Thermal Diffusivity (cm ² /sec)
36	0.17745	0.001231
39	0.19622	0.00224
140	0.31911	0.00478
238	0.33714	0.005135
259	0.45054	0.008632
323	0.49899	0.007032
385	0.60507	0.01079
428	0.4471	0.0061967
511	0.5602	0.008981
597	0.73055	0.01010
618	0.7067	0.011426
650	0.5415	0.00704
748	0.6728	0.00814
808	1.0671	0.01625

Fig. 3. Thermal Conductivity of Thomas Coke

Fig. 4. Thermal Diffusivity of Thomas Coke

Fig. 5. Thermal Conductivity of Mary Lee Coke

Fig. 6. Thermal Diffusivity of Mary Lee Coke

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THE UNIVERSITY OF ALABAMA COLLEGE OF ENGINEERING

The College of Engineering of The University of Alabama (Tuscaloosa) has an undergraduate enrollment of more than 1,000 students and a graduate enrollment of 90-100. There are approximately 100 faculty members, a significant number of whom conduct research in addition to teaching.

Research is an integral part of the educational program, and interests parallel academic specialities. It is conducted in the classical engineering programs of aerospace, chemical, civil, electrical, engineering hydrology, engineering mechanics, environmental, industrial, mechanical, metallurgical, and mineral engineering. All of these programs offer the master's degree, and five programs offer the educational specialist and doctor of philosophy degrees.

Other organizations on the University campus that contribute to particular research needs of the College of Engineering are the Charles L. Seebeck Computer Center, Geological Survey of Alabama, Marine Environmental Sciences Consortium, Mineral Resources Institute—State Mine Experiment Station, Natural Resources Center, U.S. Bureau of Mines, Tuscaloosa Metallurgy Research Center, and the Research Grants Committee.

This University community provides opportunities for interdisciplinary work in pursuit of the basic goals of teaching, research, and public service.