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**Modeling of Hydrologic Conditions and Solute Movement
in Processed Oil Shale Waste Embankments Under Simulated
Climatic Conditions**

**Quarterly Report
Third Quarter FY 1993
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1.0 Introduction

This report presents research objectives, discusses activities, and presents technical progress for the period April 1, 1993 through June 31, 1993 on Contract No. DE-FC-21-86L-C11084 with the Department of Energy, Laramie Project Office. This research is titled "Modeling of Hydrologic Conditions and Solute Movement in Processed Oil Shale Waste Embankments Under Simulated Climatic Conditions" and is the continuation of previous research initiated in 1986.

The scope of the research program and the continuation is to study interacting hydrologic, geotechnical, and chemical factors affecting the behavior and disposal of combusted processed oil shale. The research combines bench-scale testing with large scale research sufficient to describe commercial scale embankment behavior. The large scale approach was accomplished by establishing five lysimeters, each 7.3 x 3.0 x 3.0 m deep, filled with processed oil shale that has been retorted and combusted by the Lurgi-Ruhrgas (Lurgi) process. Approximately 400 tons of Lurgi processed oil shale waste was provided by Rio Blanco Oil Shale Co., Inc. (RBOSC) through a separate cooperative agreement with the University of Wyoming (UW) to carry out this study.

Three of the lysimeters were established at the RBOSC Tract C-a in the Piceance Basin of Colorado. Two lysimeters were established in the Environmental Simulation Laboratory (ESL) at UW. The ESL was specifically designed and constructed so that a large range of climatic conditions could be physically applied to the processed oil shale which was filled in the lysimeter cells.

2.0 Milestone Schedule/Progress Summary

A continuation application and proposal which outlined and described the research to be conducted was submitted to the LPO in January 1991. The proposed research program would be conducted over a two year period. Budgets were developed for the first and second years for this research and submitted as part of the proposal. The proposal was accepted by LPO and the Morgantown Energy Technology Center (METC) in April 1990. Work was initiated on the proposed research May 1, 1991 upon notification that the first year budget had been finalized by METC and UW.

The objectives of the continuation research are:

- Determine and assess effects on the hydrologic and geotechnical properties of the disposed processed oil shale waste material caused by extreme precipitation input sufficient to achieve steady state drainage of water through the oil shale waste material.
- Determine and assess effects on the hydrologic and geotechnical properties of the disposed processed oil shale caused by multiple freeze-thaw cycles and extreme storm events.

Five milestones were outlined and discussed in the continuation research plan and the previous quarterly reports for this project. A time/activity schedule and a brief discussion of progress is presented below for these milestones:

1. **Prepare an interim report presenting data and discussing conclusions accomplished for Cooperative Agreement DE-FC21-86LC11084 from October 1986 to May 1991.**

Discussion: A draft of this report was completed for both internal review and review by the COTR in December 1991. This draft is currently being revised and finalized. The final draft for this report was completed in April 1992.

Status: Completed 4/92.

2. **Design (model) a series of simulated climatic conditions and rainfall events which will provide extreme hydrologic and geotechnical conditions to the processed oil shale in the Environmental Simulation Laboratory (ESL).**

Discussion: Two climatic models were developed to accomplish the research objectives. The first climatic model and sampling program was designed to accommodate objectives for infiltration behavior, and to develop and analyze saturated conditions in the processed oil shale. The second climatic model was run after saturated conditions have been developed within the profile. This model was designed to produce a series of freeze thaw conditions and analyze the effects on the processed oil shale. A detailed discussion of the climatic models were presented in a previous quarterly report.

Schedule: 7/3/91 - 12/31/91.

Status: Completed.

3. **Apply the designed climatic conditions in the ESL and collect hydrologic and geo-technical data.**

Discussion: The environmental simulation laboratory has the capability of monitoring runoff and determining a runoff hydrograph via an automated weighing water collection system. Infiltration curves for each applied storm can be basically developed by subtracting the measured runoff hydrograph data from the applied rainfall hyetograph. Infiltration curves produced from different storm events will be evaluated as a function of the antecedent moisture content at several depths, and from the hydraulic gradients within the profile. Water contents will be measured before, during, and after all applied storm events. Hydraulic gradients will be calculated from water characteristic curves that were previously developed in this research program.

Schedule: 2/10/92 - 12/92 .

Status: Completed 3/93.

4. **Destructively sample and dispose of the processed waste material in the lysimeter beds of the ESL.**

Discussion: Destructive sampling will be conducted to extract undisturbed specimens and cores of the processed oil shale at several different depths. These specimens will be used to evaluate hydrologic properties, soil mechanical properties, and leachate chemical properties. These data obtained and the properties measured from the "weathered" processed oil shale will be compared to the results from the testing program which was previously conducted.

Schedule: 3/93 - 5/93 (rescheduled)

Status: This objective was again rescheduled. It was determined that destructive sampling was more easily accomplished during extraction of the processed oil shale from the lysimeter beds. Sampling is to be accomplished as each lift is being extracted from the lysimeter. Extraction of the material was initiated in June 1993 and is expected to continue through August 1993. These changes are shown in an updated Time/Activity Table presented in section 3.1.

5. **Analyze and evaluate all data sets and prepare final report.**

Discussion: This report will be a comprehensive report, detailing all data and results, for this Cooperative Agreement.

Schedule: Data Analysis (7/93 - 9/93) Report (10/93 - 12/93)

3.0 Technical Progress/Results

3.1 Time/Activity Schedule for Project Completion

- Application of freeze/thaw climatic model.
Schedule: August - December 1992.
Status: Completed March 1993.
- Conduct post freeze/thaw infiltration and in situ hydraulic conductivity measurements.
Schedule: January - February 1993.
Status: Completed May 1993.
- Process necessary data, information, and reports in order to meet state and federal regulatory requirements for permanent disposal of the processed oil shale.
Schedule: February - June 1993.
Status: Completed May 1993
- Develop and finalize the destructive sampling plan for the processed oil shale in the lysimeters.
Schedule: February 1993
Status: Sampling Plan was outlined and implemented in June 1993 in conjunction with extraction of the processed oil shale.
- Develop and finalize processed shale removal and disposal plan.
Schedule: March 1993
Status: Plan for removal was outlined and initiated in May 1993 in conjunction with destructive sampling.
- Conduct destructive sampling of processed oil shale to obtain cores for the measurement of hydraulic conductivity, leachate chemistry, and soil mechanical properties.
Schedule: April - May 1993
Status: Initiated in June 1993 with extraction of processed shale from the lysimeter beds. Results from these data will be completed and discussed in the next quarterly report.
- Remove processed shale from lysimeters and implement disposal according to developed plan according to all regulatory requirements.
Schedule: May - July 1993
Status: Extraction of the processed oil shale was initiated in late May 1993 and will proceed through August 1993. The extraction of the processed oil shale from the ESL has proved to be more difficult, timely, and costly than was originally estimated.
- Complete data analysis for project.
Schedule: July - September 1993
- Complete final report and close out contract.
Schedule October - December 1993

3.2 Hydrologic Modeling

Efforts to model the infiltration and movement of water through the processed oil shale test embankments were concluded during the third quarter. These efforts and much of the following discussion were adapted from a thesis by Rangarajan (1993), whose graduate research program has been done in conjunction with this project.

The variably saturated flow model program UNSAT2 was utilized to model water flow through the processed oil shale embankment. The objective of using this program was to determine if it could be used to predict infiltration, runoff, drainage, and movement of water within the test embankment.

Two sets of data were used to run the program. One set of data included in-situ saturated hydraulic conductivities measured using a Geulph permeameter and a double ring infiltrometer. For the second set of data, horizontal hydraulic conductivities from the Geulph permeameter test were used but the vertical hydraulic conductivities were determined from bench-scale tests conducted at the University of Wyoming.

Description of Model

The UNSAT2 program developed by Neuman (1974) is intended for analysis of flow in unsaturated, partially saturated, or saturated porous media. It is capable of handling flow regions delineated by irregular boundaries and composed of non-uniform soils having arbitrary degrees of local anisotropy. It can simulate flow in the vertical plane, the horizontal plane, or in three dimensional radial symmetry about the vertical axis. The program can deal with boundaries controlled by atmospheric conditions such as seepage faces, and evaporation or infiltration surfaces in addition to conventional head and flux boundaries. The program also has an unique restart feature which updates the boundary condition as well as the boundary values with time. The program utilizes the lumped-mass Galerkin finite element scheme with quadrilateral and triangular elements for solution.

The following basic flow equation which takes into account advection, drainage, storage, and source/sink terms is used to calculate water movement within the soil:

$$L(h) = \underbrace{\sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_i} \left[K^x(h) K_{ij}^s \frac{\partial h}{\partial x_j} \right]}_{\text{Advection}} + \underbrace{\sum_{i=1}^3 \frac{\partial}{\partial x_i} K^x(h) K_{i3}^s}_{\text{Drainage}} - \underbrace{[C(h) + \rho S_s] \frac{\partial h}{\partial t}}_{\text{Storage}} - \underbrace{S}_{\text{Source/Sink}} = 0 \quad (3.2.1)$$

where:

- L = quasilinear differential operator in flow region
- x_i = spatial coordinates
- K^r = relative hydraulic conductivity ($0 < K^r < 1$)
- K^s_{ij} = hydraulic conductivity tensor at saturation
- h = pressure head
- C = specific moisture capacity = $d\theta/dh$
- θ = volumetric moisture content
- β = 0 in unsaturated zone & 1 in saturated zone
- S_s = specific storage
- t = time
- S = source/sink term

UNSAT2 is also capable of accounting for plant transpiration, and a root density function reflecting root surface area per unit bulk volume of soil and some effective distance over which the water moves to the roots. To solve the basic flow equation, initial conditions within the flow region must be specified. The pressure head is assumed to be a single-valued function of the water content and hysteresis is not considered.

The numerical solution to the basic flow equation subjected to initial and boundary conditions is obtained by dividing the flow region into a network of triangular or quadrilateral elements and applying Galerkin's method to formulate and solve the element equations. The resulting approximate solution of Eq. 3.2.1 is obtained at any point in the flow region and at any time step.

The program is capable of simulating evaporation and infiltration boundaries by specifying either a prescribed head or prescribed flux boundary. The time intervals for solution are computed independently. At any time step during the first iteration, the program treats the nodes as prescribed boundaries with a flux equal to a fraction of the specified potential and slowly increases for convergence. The program also updates the pressure head and moisture content at every node at every time increment. It can treat the development of a seepage face at any stage of computation and treat the saturated nodes as a prescribed head boundary with pressure head equal to zero, indicating discharge from the porous media through saturated nodes. At the same instant, the unsaturated nodes are treated as prescribed flux boundaries with no discharge.

Computer Simulations

Processed oil shale in the ESL was placed in eight, 0.30 m (1 ft) thick lifts with a gravel drain at the bottom. The model consisted of 462 nodes and 432 elements providing a two-dimensional model of the test embankment, as shown in Figure 3.2.1. The surface of processed oil shale in the test embankment slopes gently (1 in 48) to allow collection of runoff during rainstorms and this was simulated in the model. The entire length and depth of the test embankment was used in the simulation. The model was 7.33 m (24 feet) long, 2.40 m (8 feet) deep, and 1 cm wide.

Figure 3.2.1 Two Dimensional Finite Element Mesh of the Test Embankment.

The physical property values used as input consisted of porosity, specific gravity, specific storage, and saturated horizontal and vertical hydraulic conductivities. Based on the value of specific gravity measured in an earlier study and the in-situ unit weight during placement of processed oil shale in the ESL, the porosity was computed. A constant porosity of 0.45 was assumed and input into the model. But, due to hydration and cementation, the pore spaces could have reduced and decreased porosity with time. This change was not taken into consideration during modeling. Also, the specific storage, defined as the volume of water released from storage per unit volume of saturated soil due to a unit decrease in pressure head, is dependent on the moisture content and compressibility effect. Since the compressibility effect of processed oil shale is very small, a value of one percent was assumed. Table 3.2.1 summarizes the physical properties input into the model from in-situ hydraulic conductivity measurements and from bench-scale measurements.

Modeling consisted of simulating the top surface as an infiltration face and the bottom as a seepage face. All of the surface nodes were modeled as infiltration nodes and all of the bottom nodes as seepage nodes. The other nodes were modeled as internal nodes but not as a sink or source.

Table 5.1 Physical Properties of Processed Oil Shale

Physical Property					Value
Porosity (n)					0.45
Specific Gravity (G)					2.67
Specific Storage					0.01
van Genuchten Model Parameters	α				0.00112
	n				3.70
k (cm/hr)	Material	Lift	k_h (in-situ)	k_v (in-situ)	k_v (Lab)
	#1	Top 6 in	1.55	5.34	0.11
	#2	2nd & 3rd	2.40	0.83	0.45
	#3	4th & 7th	4.45	1.04	0.45
	#4	5th & 6th	7.21	7.41	0.45
	#5	1st & 8th	12.20	5.34	0.45
	#6	Thin Element	23.90	7.81	0.45

The initial horizontal hydraulic conductivity was approximated from in-situ measurements made with the Geulph permeameter and the vertical hydraulic conductivities from measurements made with the double-ring infiltrometer. Since the horizontal hydraulic conductivity showed higher values at the interfaces than between lifts, thin elements with higher horizontal hydraulic conductivity were introduced at the interface between the lifts in the model. This resulted in six material types with different horizontal hydraulic conductivities, as shown in Table 3.2.1.

The processed oil shale was modeled for vertical plane flow. An initial moisture content of eight percent was assumed, based on measurements made after simulation of two years of climatic condition similar to that measured at test site and before applying the twenty-three rainstorms to the embankment. The soil-moisture characteristic relationship required in the simulation was obtained from pressure plate tests. The relative hydraulic conductivity (K^r) at various moisture contents required during the simulation was computed from the van Genuchten expression (van Genuchten, 1980).

The van Genuchten expression is a closed-form equation for predicting hydraulic conductivity of unsaturated soils. The expression is dependent on four independent parameters: residual water content, defined as water content at a very high capillary pressure (θ_r), water content at saturation (θ_s), and curve fitting constants (α and n) which have to be estimated from observed soil-water retention data. The curve fitting constants α and n are estimated from the absolute value of the slope of the soil-moisture retention curve.

Twenty-three rainstorms were applied to the processed oil shale embankment in the ESL. During each rain event, cumulative runoff was measured every 30 seconds. Infiltration rate was computed as the difference between the rate of applied rain and rate of runoff. A typical plot of rate of applied rainfall, measured infiltration, and runoff against time for the first applied rain event is shown in Figure 3.2.2. Each rain event and the dry period between rain events were simulated and modeled. Cumulative rainfall durations and rates, and dry period durations are summarized in Table 3.2.2.

Infiltration rate was computed at 2.5 minute time intervals. Runoff rate was calculated as the difference between the rate of rain applied to the surface and infiltration. The simulated rates of infiltration and runoff were compared to the measured rates. Figures 3.2.3 through 3.2.8 show comparisons of simulated infiltration and runoff, using in-situ measured hydraulic conductivities, to measured infiltration and runoff. Figures 3.2.9 through 3.2.18 show comparisons of simulated infiltration and runoff, using bench-scale hydraulic conductivities, to measured values. The movement of moisture during the rainstorms and also during the dry periods between rainstorms were modeled using the RESTART feature in the program. These comparisons are discussed below.

It was observed that after the tenth rainstorm the test embankment was completely saturated and started to drain into the gravel layer below. The leachate was collected and measured using collection tanks. Figure 3.2.20 shows the measured rate of drainage out of the ESL versus time for the 21st and 22nd rainstorm. The model described in this chapter was simulated such that drainage started to occur after the tenth rain event.

Figure 3.2.2 Rate of Rainfall, Computed Infiltration, and Runoff, versus Time for the Rainstorm 1.

Table 3.2.2 Rainstorm and Dry Period Duration Data

Event	Duration (hr)	Rate (cm/hr)
1st Rain	0 - 1.336	6.985
1st Dry	1.336 - 67.70	
2nd Rain	67.70 - 68.59	6.985
2nd Dry	68.59 - 164.52	
3rd Rain	164.52 - 165.97	6.985
3rd Dry	165.97 - 212.95	
4th Rain	212.95 - 214.15	7.112
4th Dry	214.15 - 259.70	
5th Rain	259.70 - 261.00	7.239
5th Dry	261.00 - 331.78	
6th Rain	331.78 - 332.97	7.620
6th Dry	332.97 - 379.96	
7th Rain	379.96 - 381.36	7.112
7th Dry	381.36 - 427.82	
8th Rain	427.82 - 429.21	7.620
8th Dry	429.21 - 500.77	
9th Rain	500.77 - 501.99	7.239
9th Dry	501.99 - 547.75	
10th Rain	547.75 - 549.00	7.239
10th Dry	549.00 - 596.23	
11th Rain	596.23 - 597.53	7.239
11th Dry	597.53 - 667.38	
12th Rain	667.38 - 668.71	7.239
12th Dry	668.71 - 716.00	
13th Rain	716.00 - 717.32	7.239
13th Dry	717.32 - 763.55	
14th Rain	763.55 - 765.12	7.239
14th Dry	765.12 - 835.42	
15th Rain	835.42 - 836.78	7.239
15th Dry	836.78 - 883.32	
16th Rain	883.32 - 884.64	7.239
16th Dry	884.64 - 931.34	
17th Rain	931.34 - 932.67	7.239
17th Dry	932.67 - 1003.10	
18th Rain	1003.10 - 1004.53	7.239
18th Dry	1004.53 - 1050.95	
19th Rain	1050.95 - 1052.37	7.239
19th Dry	1052.37 - 1171.37	
20th Rain	1171.37 - 1172.96	7.239
20th Dry	1172.96 - 1219.03	

Table 3.2.2 Rainstorm and Dry Period Duration Data (Continued)

Event	Duration (hr)	Rate (cm/hr)
21st Rain	1219.03 - 1220.24	7.239
21st Dry	1220.24 - 1267.77	
22nd Rain	1267.77 - 1269.24	7.239
22nd Dry	1269.24 - 1339.11	
23rd Rain	1339.11 - 1340.61	7.239

Figure 3.2.3 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with in-situ Measurements for the Rainstorm 1.

Figure 3.2.4 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with in-situ Measurements for the Rainstorm 2.

Figure 3.2.5 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with in-situ Measurements for the Rainstorm 3.

Figure 3.2.6 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with in-situ Measurements for the Rainstorm 4.

Figure 3.2.7 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with in-situ Measurements for the Rainstorm 5.

Figure 3.2.8 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with in-situ Measurements for the Rainstorm 6.

Figure 3.2.9 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 1.

Figure 3.2.10 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 2.

Figure 3.2.11 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 3.

Figure 3.2.12 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 4.

Figure 3.2.13 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 5.

Figure 3.2.14 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 6.

Figure 3.2.15 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 7.

Figure 3.2.16 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 8.

Figure 3.2.17 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 9.

Figure 3.2.18 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 10.

Figure 3.2.19 Comparison of Simulated Infiltration and Runoff to Measured Infiltration and Runoff with Bench-Scale Measurements for the Rainstorm 11.

Figure 3.2.20 Rate of Drainage Measured from Cell 1 versus Time.

Discussion of Modeling Results

For the first set of data where the hydraulic conductivities were input from in-situ measurements, there was no predicted runoff on the surface of the modeled embankment for the first four rainstorms as shown in Figures 3.2.3 through 3.2.7. Possible reasons for this behavior could be: (1) the numerical model computes the relative hydraulic conductivity using the van Genuchten expression as a function of water content and soil-moisture characteristics. Since the initial water content in the processed oil shale was low, the model could have overestimated the hydraulic conductivity of the processed oil shale initially. The soil-moisture characteristic curve was determined from laboratory prepared samples, these samples may not be representative of grain size distribution in the test embankments at the ESL. Hence, the van Genuchten modeling parameters is not representative of that of processed oil shale in the ESL, (2) possible overestimation of saturated hydraulic conductivity from double ring infiltrometer tests, and (3) the assumption of constant specific storage and porosity based on the bench-scale tests may not be representative of the processed oil shale in the test embankment.

The second set of data consisted of horizontal hydraulic conductivities from Geulph permeameter and vertical hydraulic conductivities from bench-scale test measurements as input. Results shown in Figures 3.2.9 through 3.2.19 indicate that numerical modeling can closely predict the infiltration and runoff during the first five rain events. But after five rainstorms, as the cumulative inflow increases, the model starts to overestimate the rate of runoff. This could be due to the fact that the bench-scale specimens undergo uniform cementation unlike large-scale embankments where aggregation could be possible. Hence, the hydraulic conductivity predicted by the bench-scale test would be much lower than the actual hydraulic conductivity measured in the full-scale embankment. It should also be noted that a constant value of porosity and specific storage is assumed in the model. In large scale embankments, however, these values may vary with time and depth. They could vary with change in water content, change in physical and chemical properties, or change in climatic conditions.

Cumulative inflow into the model is computed until the model embankment is saturated and then remains constant. The model reaches a steady state flow condition, at which point all the water applied at the surface runs off with very little infiltration. As the model embankment gets completely saturated, a seepage face develops at the lower boundary. The drainage flux at the saturated nodes slowly increases until the value reaches the rate of applied rainfall. It was observed from the applied rainstorms on the processed oil shale in the ESL that at the end of the tenth rain, the embankment was completely saturated and started to drain. It was observed from calculation of infiltration and runoff with UNSAT2 that the first simulation model was saturated at the end of the sixth rainstorm and started to drain. However, it was not possible to simulate drainage and movement of water through the embankment beyond the tenth rainstorm. The program was a poor predictor of infiltration, runoff, and drainage for this data. Whereas, for the second model using laboratory measured bench-scale data, the program was successful in predicting drainage after the tenth rainstorm but it was not possible to predict the rate of drainage through the embankment. Best predictions were obtained using bench-scale values as opposed to measured in-situ values. For better predictions of infiltration, runoff, movement of water, and drainage, a parametric

analyses needs to be done to determine the effects of different parameters, like porosity, specific storage, and van Genuchten modeling parameters used in UNSAT2.

These simulations indicate that it is difficult to model the processed oil shale in the ESL because of its changing properties with water content and climatic conditions. Simulation indicates that an accurate measurement of the soil-moisture retention curve is very important because it plays a significant role in the manner in which the program computes hydraulic conductivity using the van Genuchten modeling parameters.

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