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DP-MS-87-81

THREE-DIMENSIONAL SIMULATION OF GROUNDWATER FLOW AND TRANSPORT OF CHEMICAL AND LOW-LEVEL RADIOACTIVE CONSTITUENTS WITHIN TWO PRODUCTION AREAS OF THE SAVANNAH RIVER PLANT

by

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A paper proposed for presentation at the
Ninth Annual DOE Low-Level Radioactive Waste Management Conference
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August 25-27, 1987

and for publication in the proceedings

DP-MS-87-81

THREE-DIMENSIONAL SIMULATION OF GROUNDWATER FLOW AND TRANSPORT OF CHEMICAL AND LOW-LEVEL RADIOACTIVE CONSTITUENTS WITHIN TWO PRODUCTION AREAS OF THE SAVANNAH RIVER PLANT

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INTRODUCTION

To assist in the assessment of the impacts of waste management activities at the Savannah River Plant (SRP), modeling of transport in the environmental media was performed. Predicting the future performance of any waste site or facility and postulated actions in terms of migration of potential hazardous materials requires mathematical models capable of simulating flow and transport in the groundwater. Three-dimensional groundwater flow and transport models were developed to simulate the groundwater movement and contaminant transport in two specific production areas, the Raw Materials Fabrication Area and the Separations Area, on SRP (Figures 1 and 2). The overall objective of the analysis was to develop groundwater flow models that could be used to quantify the rate and direction of the groundwater movement from the waste sites to points of discharge.

The USGS Modular 3D model (McDonald & Harbaugh, 1984) uses the strongly implicit procedure to solve sets of simultaneous finite-difference equations that represent the groundwater flow process. The transport functions, which are the concentration or mass flux at time t due to continuous injection starting at time t', were obtained by solving the three-dimensional advection-dispersion equations using the Sandia Waste Isolation Flow & Transport (SWIFT) model (Reeves & Cranwell, 1981).

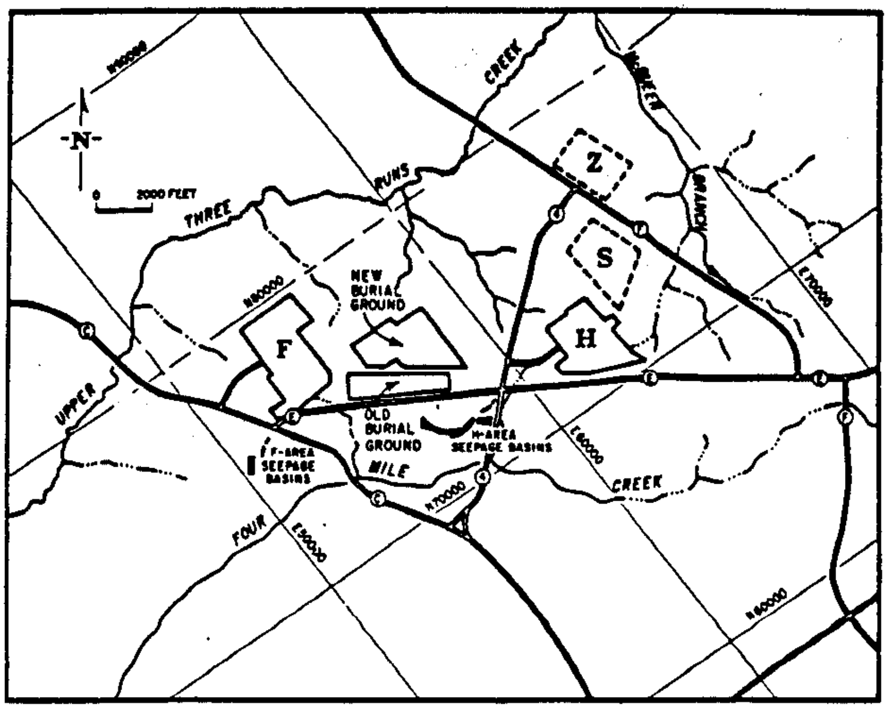

FIGURE 1. Location Map of General Separation Area, SRP

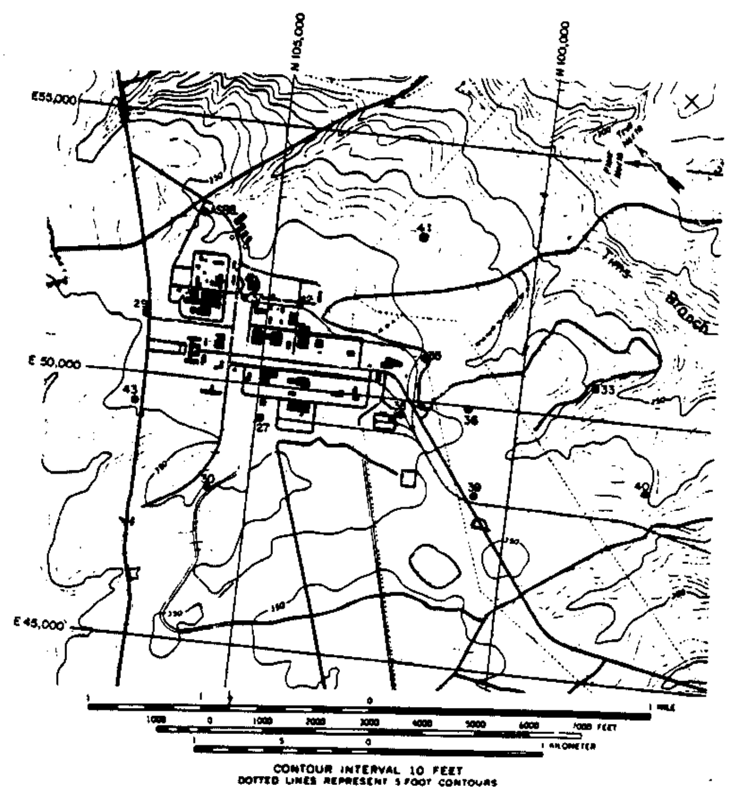

FIGURE 2. Location Map of Raw Materials Fabrication Area

CONCEPTUAL MODEL OF THE SITE AREAS

A compilation and review of the available hydrogeologic data was performed to provide the framework for the conceptual model of the sites. This information primarily included geologic data, well locations, water levels, water quality, and pumping rates for production wells.

From these data conceptual models of the groundwater flow systems were developed to generate the relevant properties and conditions of the real flow systems in a form suitable for treatment by mathematical models. The development of the conceptual model requires a knowledge of the hydrology and geology of the physical system. Simplifying assumptions were carefully selected to accommodate data uncertainties and the complex spatially and temporally variable hydrologic parameters. Boundary conditions are chosen to represent accurately the system and facilitate mathematical treatment.

The groundwater system beneath the Raw Materials Fabrication Area was divided into five hydrologic intervals, referred to as layers. This subdivision was chosen to provide a reasonable resolution of the vertical groundwater flow patterns. The selected intervals are shown in Figure 3. The areal extent of the modeled areas is shown in Figure 4 and are described in detail in S. S. Papadopulos (1986).

The conceptual model of the hydrogeologic system at the Separations Area consisted of seven hydrogeologic (four aquifers and three aquitards) units shown in Figure 5. The areal extent and finite difference grid used in the study area is detailed in Duffield et al. (1986) and shown in Figure 6.

In the conceptual models the confining layers were represented by leakance coefficients accounting for vertical conductivity and saturated thickness in the aquitards. This quasi three-dimensional approach assumes approximately horizontal flow in the aquifers and vertical flow and no storage in the confining beds.

MODEL CALIBRATION

Calibration of groundwater flow models is the process of obtaining a reasonable match between observed hydrologic data and results calculated by the numerical model. The calibration procedure was carried out by varying estimates of the hydraulic properties from a set of initial values until the best fit of calculated results to observed calibration targets was achieved.

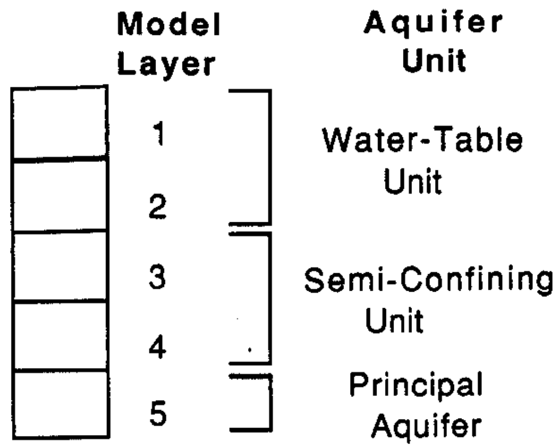

FIGURE 3. Vertical Discretization in Regional Flow Model at Raw Materials Fabrication Area

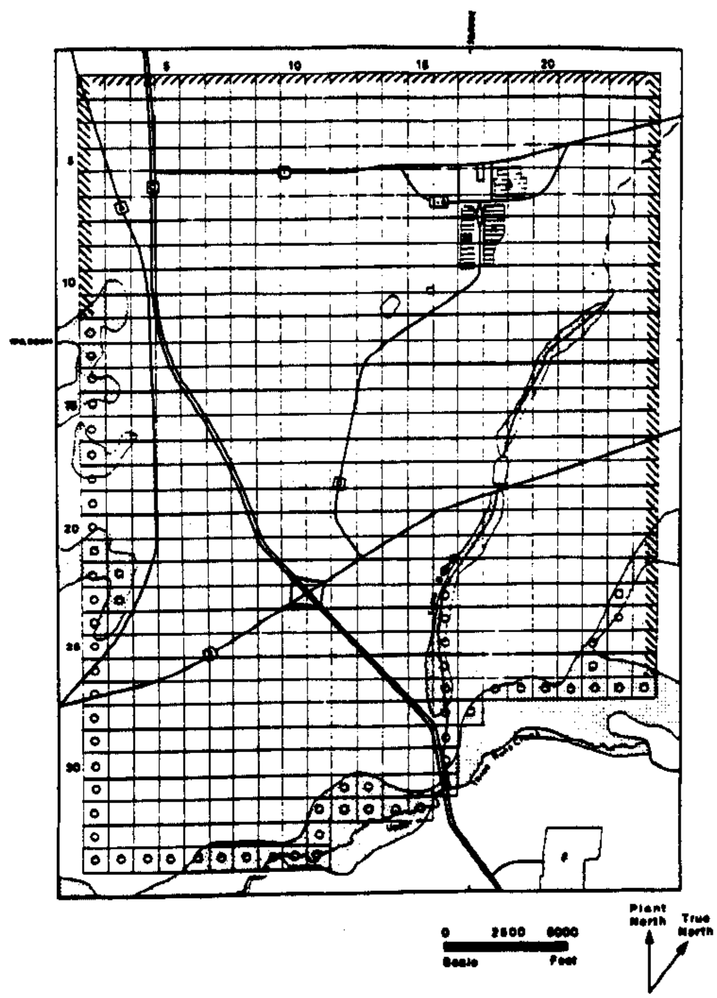

FIGURE 4. Finite Difference Grid for the Regional Flow Model at Raw Materials Fabrication Area

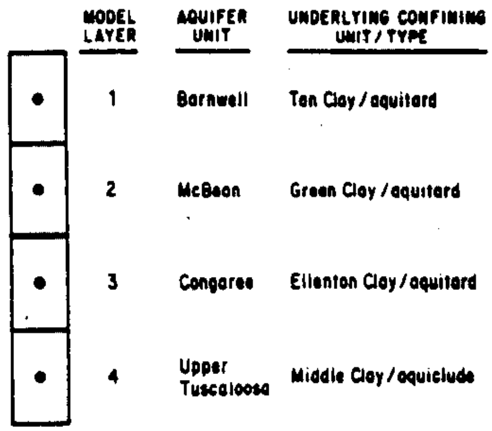

FIGURE 5. Vertical Discretization in Regional Flow Model at Separations Area

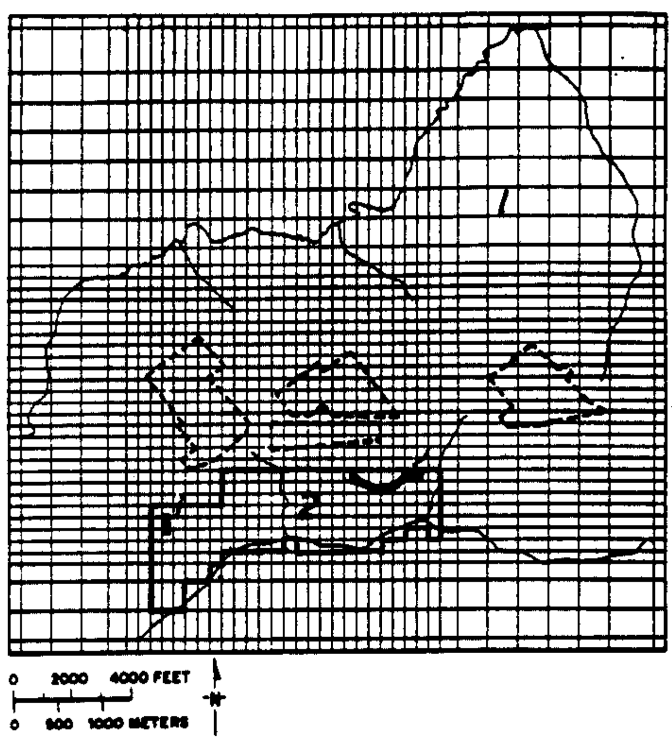

FIGURE 6. Finite Difference Grid for the Regional Flow Model at Separations Area

In this study, observed hydraulic head and stream base flow measurements were used as calibration targets. The hydraulic parameters derived from the calibration process for each layer were used in the final modeling of the flow and transport. The results of the parameter estimation for the two areas are shown in Tables 1 and 2.

RESULTS

The three-dimensional numerical models were used to determine the flow directions, velocities, and outcrop concentrations in the two specific production areas. The flow path and velocity data obtained provided information for the PATHRAE runs (analytical model use to calculate health risk from groundwater transport). Transport calculations of a few specific species were then run for comparison with the results obtained from PATHRAE.

The comparison runs were made for the two SRP locations, the Raw Materials Fabrication Area and the Separations Area. A brief description of the sites, the model input data, and example output data are described in Looney et al. (1986). The facility input parameters were defined to be common for the modeling approaches.

The results of the model comparison for selected constituents from the two areas are shown in Figure 7. Three groundwater velocities were assessed using PATHRAE to aid in data interpretation; because of the nature of the three-dimensional numerical models, the composite velocity (transport distance/transport time) varies for each receptor. In each case, the slowest velocity (V_{min}) is the velocity to the 1 m well, the highest velocity (V_{max}) is the velocity to the outcrop, and the intermediate velocity (V_{nom}) was the velocity to the 100 m well.

In all cases, PATHRAE predicted higher peak concentrations, however, the PATHRAE predictions decreased more rapidly following the peak. The concentrations were generally one to three orders of magnitude below the peak when the PATHRAE predictions first decreased below those of the numerical models. Based on these data, V_{nom} was selected for the analysis, and the outcrop distance was adjusted so that the peak would occur in the correct year. The behavior of the results is entirely consistent with expectations and the model formulations.

ACKNOWLEDGMENT

The information contained in this article was developed during the course of work under Contract No. DE-AC09-76SR00001 with the U.S. Department of Energy.

TABLE 1

Summary of Final Estimates of Hydraulic Parameters Used in the Flow Model of the Raw Materials Fabrication Area

Layer	Transmissivity (ft^2/day)	Hydraulic Conductivity (ft/day)	Leakance Coefficient $(day)^{-1}$
1	175	9	
1-2			3.5×10^{-4}
2	2,200	46	
2-3			4.0×10^{-4}
3	1,300	35	
3-4			2.7×10^{-4}
4	1,600	29	
4-5			6.0×10^{-5}
5	12,500	73	

TABLE 2

Summary of Final Estimates of Hydraulic Parameters Used in the Flow Model of the Separations Area

Layer	Transmissivity (ft^2/day)	Hydraulic Conductivity (ft/day)	Leakance Coefficient $(day)^{-1}$
1		0.8 (Zone 1) 3.6 (Zone 2)	
1-2			5.5×10^{-4} (Zone 1) 2.4×10^{-4} (Zone 2)
2		4.1	
2-3			4.4×10^{-5} (Zone 1) 1.7×10^{-5} (Zone 2)
3	3,800		
3-4			4.7×10^{-11}
4	9,810		

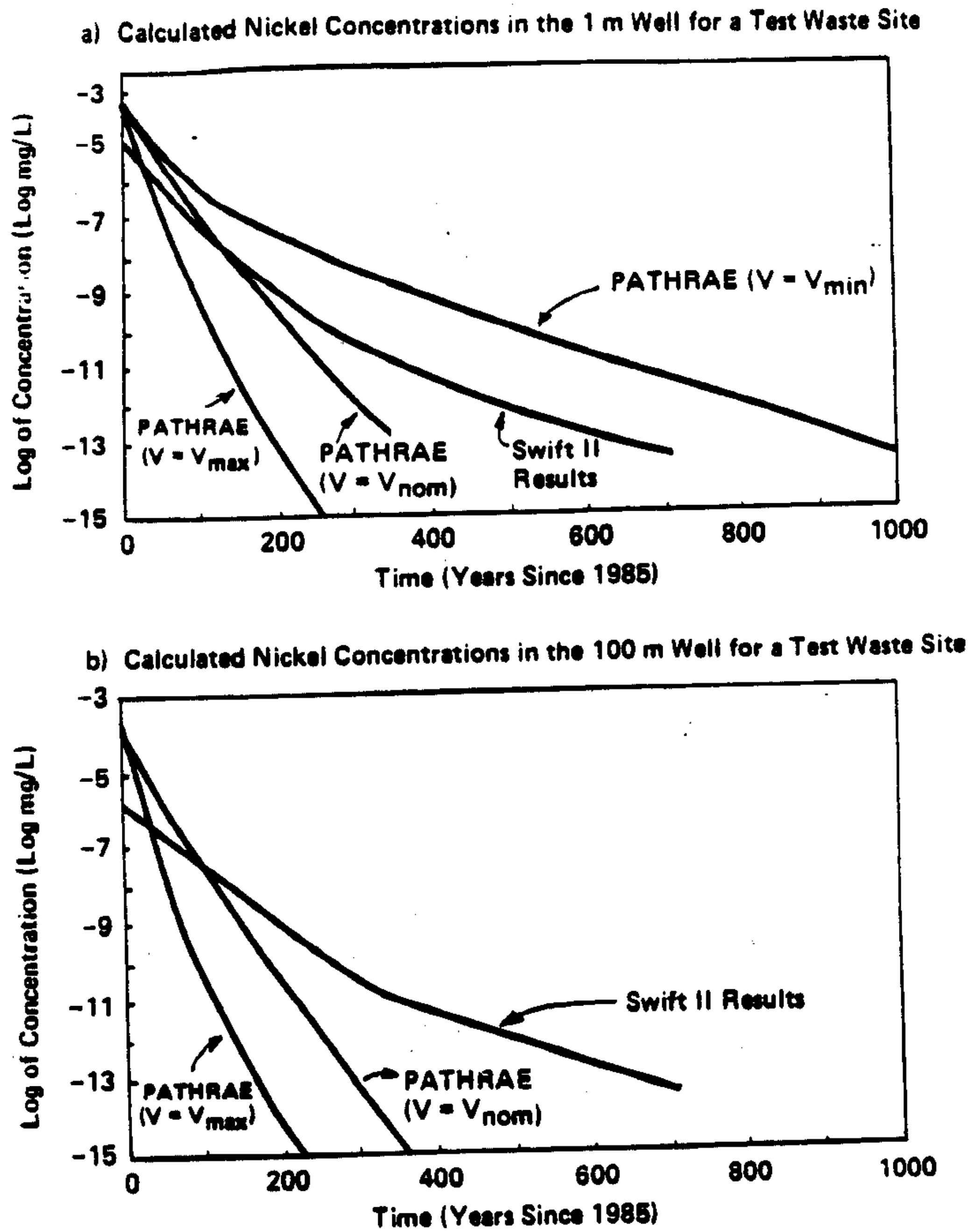

FIGURE 7. Comparison of PATHRAE Results to Multidimensional Model a) at 1 m well, b) at 100 m well. Various flow velocities were tested where $V_{min} < V_{nom} < V_{max}$, and V_{nom} was the nominal value.

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Duffield, G. M., D. R. Buss, R. W. Root, Jr., S. S. Hughes, and J. W. Mercer, 1986. **Characterization of Groundwater Flow and Transport in the General Separations Area Savannah River Plant, Flow Model Refinement and Particle-Tracking Analysis,** CORR-86-0031, Report by GeoTrans, Inc., for E. I. du Pont de Nemours and Company, Savannah River Laboratory, Aiken, SC.

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CSR 25-5
(REV 3-83)

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(TWX 810-771-2670, TEL: 803-725-6211, WU: AUGUSTA, GA.)

August 7, 1987

Ms. Marjorie Clearwater
Low-Level Waste Management Program
EG&G Idaho, Inc.
P. O. Box 1625
Idaho Falls, ID 83415

Dear Ms. Clearwater:

The camera-ready masters and one copy of each of three summary papers for the Denver conference are enclosed. The papers are: "Pathway Analysis Models Used for Assessment of Forty-Five Waste Site Areas at the Savannah River Plant" (DP-MS-87-79) by B. B. Looney, et al., "Three-Dimensional Simulation of Groundwater Flow and Transport of Chemical and Low-Level Radioactive Constituents Within Two Production Areas of the Savannah River Plant" (DP-MS-87-81) by D. E. Stephenson, et al., and "Summary of Environmental Impacts and Costs for Waste site Closure Options at the Savannah River Plant" (DP-MS-87-82) by W. F. Johnson and R. A. Moyer.

If we can be of further assistance, please let me know.

Yours very truly,

L. W. Ice

L. W. Ice, Process Editor
Site Services Department

LWI:bav
0754V

Enclosures

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W. F. Johnson, 773-42A
C. T. Sutherland, 773-A
SRL File: DP-MS-87-79
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CC: W. F. Perrin, DOE-SR (2)
R. J. Guschl, 773-A
J. C. Corey-D. E. Gordon, 773-A
D. E. Stephenson-B. B. Looney, 773-42A
File: (DP-MS-87-81)

July 21, 1987

Mr. J. R. Powell, Technical Information Officer
U. S. Department of Energy
Savannah River Operations Office
Aiken, SC 29801

Dear Mr. Powell:

REQUEST FOR APPROVAL TO RELEASE SCIENTIFIC/TECHNICAL INFORMATION

The attached document is submitted for your approval for external release. Please complete Part II of this letter and return the letter to the undersigned, by: ASAP Patent clearance is requested and received via direct communication between DOE Patent Counsel and AED Patent Reviewer. The document has ~~not~~ been reviewed for classification and UCNI. The document is ~~classified~~/unclassified and contains no UCNI. (Strike words that do not apply.)

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DP-MS-87-81, "THREE-DIMENSIONAL SIMULATION OF GROUNDWATER FLOW AND TRANSPORT OF CHEMICAL AND LOW LEVEL RADIOACTIVE CONSITITUENTS WITHIN TWO PRODUCTION AREAS OF THE SAVANNAH RIVER PLANT", By D. E. Stephenson, B. B. Looney, C. B. Andrews, and D. R. Buss.

A paper proposed for presentation at the Ninth Annual DOE Loe-Level Radioactive Waste Management Conference on August 25-27, 1987 in Denver, Colorado.

Technical questions pertaining to the contents of this document should be addressed to the author(s) or

J. C. Corey, Research Manager
Environmental Sciences Division
Savannah River Laboratory

Questions concerning processing of this document should be addressed to the AED Classification Officer & Patent Reviewer at Extension 52606.

II. DOE-SR ACTION Date Received by TIO 7/21/87

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DP REPORT ☐ PAPER ☒

DP CATEGORY

AUTHOR(S) D. E. Stephenson, B. B. Looney, C. B. Andrews, and D. R. Buss

TITLE "Three-Dimensional Simulation of Groundwater Flow and Transport of Chemical And Low Level Radioactive Constituents within Two Production Areas of the Savannah River Plant"

DIVISION Savannah River Laboratory - Environmental Sciences Division

MANUSCRIPT APPROVAL

Route in turn to

	Initials	Date		Initials	Date
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CLASSIFICATION GUIDE TOPICS

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Topic 209.15.3.1

PATENT CONSIDERATIONS

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CLOSEST PRIOR ART N/A

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DATES August 25-27, 1987

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AUTHOR(S) D. e. Stephenson, B. B. Looney, C. B. Andrews, and D. R. Buss

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July 21, 1987

Mr. A. F. Westerdahl, Chief
Patent Branch
U. S. Department of Energy
Aiken, South Carolina 29808

Dear Mr. Westerdahl:

REQUEST FOR PATENT REVIEW

Please review for patent matters:

DP-MS-87-81, "THREE-DIMENSIONAL SIMULATION OF GROUNDWATER FLOW AND TRANSPORT OF CHEMICAL AND LOW LEVEL RADIOACTIVE CONSITITUENTS WITHIN TWO PRODUCTION AREAS OF THE SAVANNAH RIVER PLANT", By D. E. Stephenson, B. B. Looney, C. B. Andrews, and D. R. Buss.

A paper proposed for presentation at the Ninth Annual DOE Loe-Level Radioactive Waste Management Conference on August 25-27, 1987 in Denver, Colorado.

Please telephone your comments to the Records Management Office (Ext. 52606) and notify me by signing and returning to C. J. Banick the original of this letter. A copy is provided for your file.

If you decide to pursue a patent on any development covered, I shall be happy to supply additional information required such as appropriate reference and the names of persons responsible for the development.

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Document(s): DP-MS-87-81

Title(s): "THREE-DIMENSIONAL SIMULATION OF GROUNDWATER FLOW AND TRANSPORT OF CHEMICAL AND LOW LEVEL RADIOACTIVE CONSITITUENTS WITHIN TWO PRODUCTION AREAS OF THE SAVANNAH RIVER PLANT"

Author(s): D. E. Stephenson, B. B. Looney, C. B. Andrews, and D. R. Buss

Contractual Origin: DE-AC09-76SR00001

Present Classification: Unclassified Paper

References:

No items were noted that, in my opinion, should be called to the attention of the DOE for patent consideration.