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- 1 -

Douglas K. Vogt
CorSTAR
7315 Wisconsin Avenue
North Tower, Suite 702
Bethesda, Maryland 20814

SUBJECT: REVIEW COMMENTS ON REVISED BENCHMARK PROBLEMS FOR REPOSITORY SITING MODELS

Dear Mr. Vogt:

This letter summarizes comments and recommendations arising from the review of the above named report, received for review on July 6, 1984. This report is a revision of the previously reviewed and published report, "Benchmark Problems for Repository Siting Models", (NUREG/CR-3097, December 1982). It reflects the need for further defining benchmark problems after using them for testing and evaluating repository siting codes that was anticipated in the foreword to NUREG/CR-3097. Consequently, the review centered on those portions of the document that were modified after exercising selected codes under Tasks 4 and 5 for Repository Siting Codes.

1. An additional paragraph or two on the groundrules for using the benchmark problems should be inserted near the end of Section 2.2. It should warn that no special (i.e. " trick") techniques should be used in running the codes for test purposes and that modifications to the code should be done only as a last resort, with ample documentation.

2. It should also be noted that some problems were chosen because they had analytical solutions and provide a rigorous test of the code. A code that does not meet this test may or may not be suitable for application to HLW repository problems. That is, a code may do relatively poorly in simulating a fast transient such as a well-drawdown, but may still be adequate for the very slow transient encountered in HLW repositories. This proviso should be mentioned in Section 2.2 and in the special comments section of the specific problem write-ups to which it applies.

3. In the second paragragh of Section 4.3, Input Specifications, the authors imply that the Reeves-Duguid curve cannot be supported. Why not delete the simulation curve from Figure 4.8?

4. The evaluation of equations 5.3 and 5.7 would be quite difficult. If the results are available, they should be included.

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5. In Section 5.3, the last paragraph may not apply to all codes. For example, particle tracing codes such as Method of Characteristics can work well for purely advective problems, without dispersion.

6. In Section 8.1, Assumptions, the assumption that the domain is semi-infinite is not consistent with the E3 exit boundary condition option (Equation 8.3b).

7. In Section 8.1, Input Specifications, for Peclet number, P1, the authors intended to set Pe equal to infinity. However, INTRACOIN gave two values for the Peclet number, P1, (Pe=1,000 or infinity). The reason for this is important. The value of 1000 requires a dispersion length of 0.5m rather than the zero dispersion appropriate for a Pe of infinity. The use of a dispersion length of zero rather than 0.5m may impose undue restrictions on certain codes. (See draft report, "Benchmarking of Flow and Transport Codes for Licensing Assistance", Section 3.7).

8. In Section 8.3, Input Specifications , a single value for dispersion length is reported; however, INTRACOIN problem two has different dispersion lengths in the three zones (α_L= 5.0m, 10.0m, 35.0m).

9. In Section 9.0, boundary conditions were added to the porous medium INTRACOIN problem, but none were added for the fractured medium problem. Are they needed?

10. Please ensure that the entire document is thoroughly edited. In many cases, there are typographical errors and omitted greek letters and symbols on the re-typed pages. Examples are included in the attached markups (Enclosure 1).

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The action taken by this letter is considered to be within the scope of the current contract NRC-02-81-026. No changes to cost or delivery of contracted products are authorized. Please notify me immediately if you believe this letter would result in changes to cost or delivery of contract products.

Sincerely,

"ORIGINAL SIGNED BY"

Pauline P. Brooks
Repository Projects Branch
Division of Waste Management
Office of Nuclear Material
Safety and Safeguards

Enclosure: Markup pages
cc: Peter Cukor
Sharon Wollett

Record Note: This review was accomplished with the technical assistance of R. Codell and T. McCartin.

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ENCLOSURE

1.3 PROCESSES CONSIDERED

Only repository site evaluation is considered in this report. The processes that are important in this evaluation are (1) saturated ground-water flow, (2) unsaturated flow, (3) heat transport, and (4) solute transport. The most important of these processes are probably saturated ground-water flow and solute transport. The unsaturated zone will also be important if repositories are placed above the water table. Heat transport is considered, but this area will be covered in more detail under the repository design category. These qualitative guidelines played a role in determining how many problems were selected under each process.

The test problems that are described in this report are divided according to the processes considered. The sections are presented in the following order: (1) saturated flow, (2) unsaturated flow, (3) heat transport, and (4) solute transport. Some of the problems consider different types of media, such as porous and/or fractured.

1.4 PREVIOUS WORK

The proceeding task of simulating selected problems from this report using numerical codes selected by the NRC is under way. Initialization of the modeling task has demonstrated the expected need for further definition of the benchmark problems since their original write-up in the December, 1982 NUREG CR-3097. Hence this rewrite of that report. The forthcoming modeling work, and the previous studies described following, will provide additional basis for comparing problem solution. S

Several recent and ongoing studies have focused on testing and benchmarking codes. These include a comparison of codes at the Gordon Research Conference on Fluids in Permeable Media held July 28 - August 1, 1980. Several petroleum engineering codes applied to a three-dimensional black-oil reservoir simulation problem were compared. The results of this simulation were later published by Odeh (1981).

At the Sixth Annual Workshop on Geothermal Reservoir Engineering held at Stanford University on December 16-18, 1980, a Model Intercomparison Study was presented. The Department of Energy sponsored this study, which consisted of applying several two-phase geothermal codes to a set of benchmark problems. The results of this study were subsequently published in a Stanford University report (Stanford, 1980).

Benchmark problems have also been designed for the related area of ground-water problems associated with hazardous waste. For example, a set of test problems was assembled for the Environmental Protection Agency and is presented in Mercer et al. (1981). Only one code was used in this study, as the main goal was to develop a set of problems.

There are two current studies concerned with benchmarking codes. The Swedish Nuclear Power Inspectorate (Statens Karnkraftinspektion) is directing one of these studies, termed INTRACOIN. This study's primary focus is radionuclide transport codes. The INTRACOIN code intercomparison is performed at three levels to describe:

where T is the temperature in the aquifer, T_1 is the temperature of the injected fluid, and T_0 is the ambient temperature. For this use, the Darcy velocity can be determined by $v = Q/2\pi rb$.

The governing equations are solved subject to the following initial and boundary condition:

$$u(r,0) = 0 \quad \text{for } r > 0$$

$$u(0,t) = 1 \quad \text{for } t > 0$$

$$\lim_{r^2+z^2\to\infty} u = 0$$

Objectives. The purposes of this problem are to (1) verify the correctness and accuracy of the solution algorithm for transient heat flow, (2) to verify the solution algorithm for a cylindrical coordinate system, (3) to verify the numerical approximation logic for convection and conduction in the aquifer and (4) assess the importance of heat transfer in the confining bedrock.

Analytical Solutions. Avdonin (1964 presents an analytical solution for equations 5.1a and 5.1b:

$$u(\omega,\tau) = \frac{1}{\Gamma(\nu)}\left[\frac{\omega^2}{4\tau}\right]^{\nu}\int_0^1 \left\{\exp\left(-\frac{\omega^2}{4\tau s}\right)\operatorname{erfc}\left(\frac{\alpha s\sqrt{\tau}}{2\sqrt{1-2}}\right)\right\}\frac{ds}{s^{\nu+1}} \qquad (5.3)$$

?

S

where

$$\nu = \frac{Qc_w\rho_w}{4\pi bK_m}, \quad \omega = \frac{2r}{b}, \quad \tau = \frac{4K_m t}{c_m\rho_m b^2}, \quad \alpha = \left(\frac{K_R c_R\rho_R}{K_m c_m\rho_m}\right)$$

A

and $\Gamma(\nu)$ is the Euler's gamma function.

Assumptions. The assumptions invoked in solving the above equations include:

- Equation parameters such as porosity, heat capacity, thermal conductivity, thickness, and density are constant.
- The injection rate is uniform, and steady-state flow conditions exist in the formation. The velocity is a result of the injection only and does not consider regional flow.
- The areal extent of the formation is infinite.
- Convection and conduction in the formation are negligible in the vertical direction.

4.0 UNSATURATED FLOW

Flow in the unsaturated zone is more difficult to model than flow in the saturated zone. The principal reason for this is the dependence of the transmission of water through a partially saturated medium on the degree of saturation. This causes the governing equations to be non-linear.

As a result of non-linearities, there is a general lack of analytic solutions for fluid flow in unsaturated zones. Therefore, the problems presented here involve comparisons with semi-analytical solutions and numerical simulations of field cases.

4.1 HORIZONTAL UNSATURATED FLOW (Philip, 1955)

Problem Statement. A semi-infinite horizontal tube of soil is partially saturated with ground water (Figure 4.1). At time zero, one end of the tube is wetted, raising the water content to saturation. The flow of water along the tube is to be calculated.

The governing equation for one-dimensional flow in unsaturated media may be written in the form

$$\frac{\partial}{\partial x}\left(D\frac{\partial \theta}{\partial x}\right) = \frac{\partial \theta}{\partial t} \qquad (4.1)$$

where θ is moisture content and D is the soil-moisture diffusivity. The coefficient D is a non-linear function of θ and is defined as

$$D = Kk_r \frac{d\psi}{d\theta} \qquad (4.2)$$

where K is the saturated hydraulic conductivity, k_r is the relative permeability, and ψ is the pressure head.

The solution of equation 4.1, subject to the following initial and boundary conditions (Figure 4.2),

$$\theta(x,0) = \theta_n$$

$$\theta(0,t) = \theta_o$$

$$\theta(\infty,t) = \theta_n$$

describes the movement of moisture in a tube of soil depicted in Figure 4.1.

Objectives. The purpose of this problem is to verify the ability of a code to accurately track a propagating wetting surface.

Note that K_m and $\rho_m c_m$ can be computed using

$$K_m = \phi K_w + (1-\phi) K_r \text{ and} \tag{5.4}$$

$$\rho_m c_m = \phi \rho_w c_w + (1-\phi) \rho_r c_r \tag{5.5}$$

Output Specifications. The output for this problem includes:

(1) temperature versus radial distance at 10^9 seconds and
(2) temperature versus time at a radius of 37.5 meters

For two cases, one in which thermal conduction in the confining bedrock is taken into account, and another in which this thermal conduction is neglected.

Special Comments. Coarse grid spacing or large time steps can lead to numerical dispersion.

5.1b: LINEAR HEAT TRANSPORT DURING INJECTION

Problem Statement. The problem concerns one-dimensional movement of the thermal front in a confined aquifer that is injected with water having a temperature different from the ambient temperature (See Figure 5.2). Both conduction and convection are considered in the aquifer and only conduction is considered in the overlying and underlying bedrock. This problem is similar to 5.1a, but utilizes a linear flow field with uniform velocities.

The problem may be described by the following equations:

$$K_m \frac{\partial^2 u}{\partial x^2} - v_w \rho_w c_w \frac{\partial u}{\partial x} = \rho_m c_m \frac{\partial u}{\partial t} \tag{5.6a}$$

in the aquifer, and

$$K_R \frac{\partial^2 u}{\partial z^2} = \rho_R c_R \frac{\partial u}{\partial t} \tag{5.6b}$$

in the overlying and underlying bedrock, where all of the symbols are as defined in problem 5.1a.

The governing equations are solved subject to the folowing initial and boundary conditions:

$$u(x,z,t=0) = 0$$

$$u(x,0,t) = 1$$

- Convection does not occur and conduction is negligible in the horizontal direction in the rocks overlying and underlying the formation.

- The extent of the confining beds is infinite.

- Flow is radial.

- Dispersion can be neglected and buoyancy forces are negligible compared to forced convection.

Input Specification. Water at 160°C is injected into the fringe of a geothermal reservoir of temperature 170°C. This problem looks at one well and assumes that a quasi steady-state flow field is set up very rapidly. The velocity field is established by using, or approximating, the analytical solution $v = Q/2\pi rb$. For heat transport, the temperature at the outer radius is 170°C. Additional physical parameters are as follows:

Parameter	Value
Radius of well, r_w	0 m
External radius, R_o	600 m
Thickness of aquifer, b	100 m
Well injection rate, Q_I	0.01 m^3/sec
Injection temperature, T_I	160°C
Initial temperature, T_0	170°C
Effective porosity, ϕ	0.2
Density of water, ρ_w	1000 kg/m^3
Heat capacity of water, c_w	4180 J/kg°C
Thermal conductivity of water, K_w	0.67 W/m°C
Density of aquifer rock, $_r$	2500 kg/m^3
Heat capacity of aquifer rock, c_r	1000 J/kg°C
Thermal conductivity of aquifer rock, K_r	20 W/m°C

Thermal properties of confining bedrock may be assumed to be identical to those of the aquifer rock.

8.0 SOLUTE TRANSPORT IN SATURATED POROUS MEDIA

The transport of dissolved contaminants in saturated porous media involves the processes of advection, dispersion, and sorption. Advection is the transport of contaminants along with moving ground water. Dispersion is the spreading of contaminant pulses. Sorption is a general term describing chemical reactions with rocks and soils, which slow the transport of solutes. These processes are described by the advection-dispersion equation, also known as the solute transport equation. In this equation, the ground-water velocity appears as a parameter. Therefore, for modeling of solute transport ground-water velocity must be calculated by using a flow model. Ground-water velocity is specified in problems 8.1 through 8.4, and problems 8.5 and 8.6 use velocity fields calculated by solving problems in other sections.

Problems 8.1 through 8.4, as well as 9.1 and 9.2, have been taken from the International Nuclide Transport Code Intercomparison Study (INTRACOIN). The INTRACOIN project is an effort to benchmark a number of solute transport codes by having them run by their developers or present users against the same problems. The project is described in INTRACOIN (1981) and INTRACOIN (1982); results of problems 8.1, 8.2, 8.3, 9.1, and 9.2 will be described in a report scheduled to be published in late 1982. Inclusion of the INTRACOIN problems allows us to take advantage of their work in carefully specifying problems which test as many aspects of the codes as possible. Additional use of the ~~INTERCOIN~~ INTRACOIN problems will permit direct comparison of NRC and INTRACOIN benchmark results.

Most of the problems in Sections 8 and 9 involve decay chains. Although many of the codes to be tested do not incorporate chain decay, such codes can nevertheless be tested with the included problems by modeling transport of only the first chain member. If the code does not incorporate radioactive decay, the code results should be corrected by multiplying all results by $e^{-\lambda t}$, where λ is the radioactive decay constant and t is time. By this procedure, Problem 8.1, for example, reduces to the well-known solution of one-dimensional solute transport by Ogata and Banks (1961).

8.1 ONE-DIMENSIONAL ADVECTION WITH CHAIN DECAY, CONSTANT MIGRATION PARAMETERS

Problem Statement. This problem is concerned with one-dimensional transport of a decay chain of three radionuclides through a confined aquifer (see Figure 8.1). Physically this problem might describe contaminant transport from a rectilinear channel, as depicted in Figure 8.1, into a horizontal aquifer of large aerial extent.

B2: Prescribed solute mass flux

$$F_r(0,t) = \frac{I_r(t)}{T} \quad , \quad 0 \le t \le T \tag{8.2c}$$

$$F_r(0,t) = 0 \quad , \quad t \ge T \tag{8.2d}$$

Exit boundary condition options

E1: Semi-infinite extent

$$c_r(\infty,t) = 0 \tag{8.3a}$$

E3: Finite system of length L

$\frac{\partial c_r}{\partial x}$?

$$\frac{\partial r_c}{\partial x}(L,t) = 0 \tag{8.3b}$$

where ϕ is the effective porosity, F is the flow cross-sectional area, T is the leach duration, and $I_r(t)$ is the total inventory of nuclide r at time t. The function $I_r(t)$ satisfies Bateman's differential equation,

$$\frac{d}{dt} I_r(t) = - \lambda_r I_r(t) + \lambda_s I_s(t) \tag{8.4}$$

Should this be $I_r = 0$?

with given initial values of $I_r{}^0$.

Objectives. The problem specification includes two different decay chains, two sets of retardation factors, and three values of dispersivity. In this way, the problem tests a number of conditions which can cause numerical problems in codes, including large and small Peclet numbers, decay daughters which move much faster or much slower than parents and have much longer or shorter half-lives, and daughter nuclides with half-lives comparable to their transit times.

Analytical Solution. The solution of this problem for any species i is given by Harada et al. (1980) as

$$c_i(z,t) = N_i^S(z,t;B_{ij}) - N_i^S(z,t-T;B_{ij}e^{-\lambda_j T}) \tag{8.5}$$

Ground-water velocity, v = 1 m/yr

Porosity, ϕ = 0.01

Cross-sectional area of flow, F = 100 m^2

T2: Leach duration, T = 10^5 yr

Peclet number Pe = L/α_L

P1: Pe = ∞, α_L = 0 m

P2: Pe = 10, α_L = 50 m

P3: Pe = 1, α_L = 500 m

What relevance does this have in a system of 500m length?

Both inventories, I_1 and I_2, and both sets of retardation factors, R_1 and R_2, found in Appendix A should be used.

Output Specifications. The desired outputs are the rates of flow of the three nuclides past the point z = 500 meters.

8.2 HYPOTHETICAL TWO-DIMENSIONAL MIGRATION BETWEEN INJECTION AND WITHDRAWAL WELLS WITH CHAIN DECAY

Problem Statement. Two wells are drilled into a homogeneous aquifer with water being injected into one well at a constant rate and withdrawn from the other at the same rate. A decay chain of three radionuclides is injected as a "band release" along a line segment perpendicular to the line between the wells (see Figure 8.2). Both longitudinal and transverse dispersion occur.

Solute transport is described by the multi-dimensional advection-dispersion equation

$$B_r \frac{\partial c_r}{\partial t} = \frac{\partial}{\partial x_i} D_{ij} \frac{\partial c_r}{\partial x_j} - v_i \frac{\partial c_r}{\partial x_i} - B_r \lambda_r c_r + B_r \lambda_s^r c_s \tag{8.10}$$

Here D is the coefficient of convective dispersion, which is assumed to have its principal axes aligned in the direction of the water velocity v. B_r is the retardation factor, λ_r is the radioactive decay constant, and λ_s^r is the production rate of nuclide r from decay of nuclide s. The subscripts i and j refer to the three Cartesian coordinates and are summed when repeated. The subscripts r and s identify individual radioactive species and are not summed. The remaining symbols are as defined in Problem 8.1.

Water flows are given by the solution to Section 5.3. Wastes are transported in both aquifers toward the river at the eastern boundary.

<u>Assumptions</u>. In addition to the assumptions listed in Section 5.3, the principal assumptions made are:

- The contaminants initially have zero concentration in the river at the eastern boundary. There is no dilution when contaminants discharge into the river.
- Sorption is represented as equilibrium ion exchange.
- The contaminant source has infinitesimal vertical thickness.

<u>Input Specifications</u>. The ground-water flows are as specified in Section 5.3 (including data taken from Section 3.5). The inventory of the nuclides is I_1, given in Appendix A. Other transport parameters are as follows:

Duration of release: $T = 10^5$ yr
Effective porosity:
- Aquifers - 0.1
- Aquitard - 0.01
- Crush zone - 0.1
- Ancient river bed - 0.3

Dispersivity:
- Basalt aquifers - 100 m
- Aquitard - 10 m
- Crush zone - 10 m
- Ancient river bed - 20 m

Retardation factors (see Appendix A):
- Basalts - R_1
- Ancient river bed - R_2

<u>Output Specification</u>. The desired output is the discharge rate of each nuclide to the river. The total discharge rate should be summed over the entire length of the river and given as a function of time. Also, at the time of peak total discharge, the discharge rate per unit length along the river should be given as a function of position.

<u>Special Comments</u>. This problem has not yet been simulated. Specifications may have to be altered to ensure desired physical behavior. In particular, changes may be needed to ensure that both aquifers are contaminated and that releases to the river occur within a reasonable length of time.

See Sections 4.10 & 4.5 of Bench-marking Report.

Transport codes that cannot accommodate dynamic ground-water flows should solve the same problem using the static flow from Section 3.5.

8.5 HYPOTHETICAL SALT REPOSITORY

<u>Problem Statement</u>. This problem consists of calculating the transport of a three-member chain of radionuclides from the hypothetical salt repository described in Sections 3.6, 5.4, and 7.1.

with

$$N_1^s(z,t) = B_{11}E(1,1;1) \tag{8.6a}$$

$$N_2^s(z,t) = \sum_{j=1}^{2} B_{2j}E(j,j;2) + \frac{B_{11}\lambda_1}{v_1(\Lambda_{12}-\lambda_1\Gamma_{12})}[E(1,1;2)-E(1,1;1)+E(1,2;1)-E(1,2;2)] \tag{8.6b}$$

$$N_3^s(z,t) = \sum_{j=1}^{3} B_{3j}E(j,j;3) + \frac{\lambda_2}{v_2} \sum_{j=1}^{2} \frac{B_{2j}}{\Lambda_{23}-\lambda_j\Gamma_{23}}[E(j,j;3)-E(j,j;2)+E(2,3;2)-E(2,3;3)]$$

$$+ \frac{\lambda_1\lambda_2 B_{11}}{v_2 v_1} \sum_{j=1}^{3} [\frac{E(1,1;j)}{(\Lambda_{kj}-\lambda_1\Gamma_{kj})(\Lambda_{\ell j}-\lambda_1\Gamma_{\ell j})} + \frac{\Gamma_{kj}E(k,j;j)}{(\Lambda_{kj}-\lambda_1\Gamma_{kj}\ (\Gamma_{\ell j}\Lambda_{kj}-\Gamma_{kj}\Lambda_{\ell j})}$$

$$+ \frac{\Gamma_{\ell j}E(\ell,j;j)}{(\Lambda_{\ell j}-\lambda_1\Gamma_{\ell j})(\Gamma_{kj}\Lambda_{\ell j}-\Gamma_{\ell j}\Lambda_{kj})}]$$

$$(k < \ell,\ k \neq j,\ \ \ell \neq j;\ \ell,k = 1,\ 2,\ 3) \tag{8.6c}$$

$$\Lambda_{kj} = \frac{\lambda_k}{v_k} - \frac{\lambda_j}{v_j}\ , \quad \Gamma_{kj} = \frac{1}{v_k} - \frac{1}{v_j} \tag{8.7a}$$

$$\beta_{ij} = \begin{cases} \lambda_i\ , & i=j \\ \Lambda_{ij}/\Gamma_{ij}\ , & i \neq j \end{cases} \tag{8.7b}$$

$$\gamma_{ijk} = 1 + 4\kappa(\lambda_k - \beta_{ij})/v_k \tag{8.7c}$$

$$B_{ij} = \sum_{m=1}^{j} N_m^0 \left(\frac{1}{\lambda_i} \prod_{r=m}^{i} \lambda_r\right) \Bigg/ \prod_{\substack{\ell=m \\ \ell \neq j}}^{i} (\lambda_\ell - \lambda_j) \tag{8.7d}$$

$$v_i = v/B_i \tag{8.7e}$$

$$N_i^0 = \frac{I_i(0)}{T} \tag{8.7f}$$