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Mass Balance Computation in SAGUARO

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Mass Balance Computation in SAGUARO

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ABSTRACT

This report describes the development of the mass balance subroutines used with the finite-element code, SAGUARO, which models fluid flow in partially saturated porous media. Derivation of the basic mass storage and mass flux equations is included. The results of the SAGUARO mass-balance subroutine, MASS, are shown to compare favorably with the linked results of FEMTRAN. Implementation of the MASS option in SAGUARO is described. Instructions for use of the MASS option are demonstrated with three sample cases.

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1.0 INTRODUCTION

The finite-element code, SAGUARO (Eaton, Gartling, and Larson, 1983), has been used extensively to model groundwater flow in the partially saturated porous media region near a proposed nuclear waste repository site.* In modeling these types of problems, transient water fluxes are calculated for very long time periods. The accuracy of these long-time calculations cannot be directly verified by experiments or by comparison with analytic solutions as a result of the complexity of the problems attempted. Hence, as an indicator of the accuracy of the hydrologic solution, mass-balance routines have been written and incorporated into the SAGUARO code. These routines allow the user to specify regions, not necessarily contiguous regions, over which to calculate the mass balance by listing the grid elements making up that region. The exterior boundary sides for mass-flux calculations are then automatically determined from this element list.

The mass-balance calculation includes: (1) computation of the total mass stored within the specified region at the current time, (2) the mass flux through all the specified boundary sides, (3) the change in the mass stored in the specified region during the last time step, and (4) the net mass gain in the region, which is the difference between the change in mass

*The Nevada Nuclear Waste Storage Investigations Project, managed by the Nevada Operations Office of the U. S. Department of Energy, is examining the feasibility of siting a repository for high-level nuclear wastes at Yucca Mountain, on and adjacent to the Nevada Test Site. This work was funded in part by the NNWSI Project. The ultimate use of this information will be to develop appropriate criteria for design of subsurface facilities and for performance assessments of the site.

stored and the mass flux through the boundaries. A zero net mass gain indicates perfect conservation of the calculated mass.

The first section of this report is a brief description of the equations and techniques used to derive the mass-balance equations. Next is the definition of the input to the program necessary to implement the MASS options. The third section shows results from three test problems selected to demonstrate the use of SAGUARO's MASS command and test the mass-balance equation implementation.

2.0 FORMULATION OF MASS BALANCE EQUATIONS

The mass-balance procedure contains two calculations for a given time step: (1) calculation of the total mass stored within the specified region, and (2) calculation of the mass flux through the region boundary during this time step.

2.1 Total Stored Mass

The region for calculation of stored mass is specified by a user-defined input list (see Subsection 2.2). The total mass stored at time t for each element in this region is calculated by

$$m_s = \int \rho_f \theta dA \quad (1)$$

where ρ_f is the liquid density and θ is the volumetric moisture content (volume of water / total unit volume). To evaluate this integral over a region dA , the moisture content is expressed in terms of the finite-element shape functions, θ^T , and calculated moisture contents at node points at specific times, $\theta(x,y,t)$. The area dA is evaluated using the Jacobian, J , and the normalized natural coordinates s and t for the element. Therefore,

$$\theta = \theta^T \theta(t) \quad (2)$$

and

$$dA = |J| ds dt. \quad (3)$$

SAGUARO uses the Boussinesq approximation, which states

$$\rho_f = \rho_o(1-g\beta\Delta T) \quad (4)$$

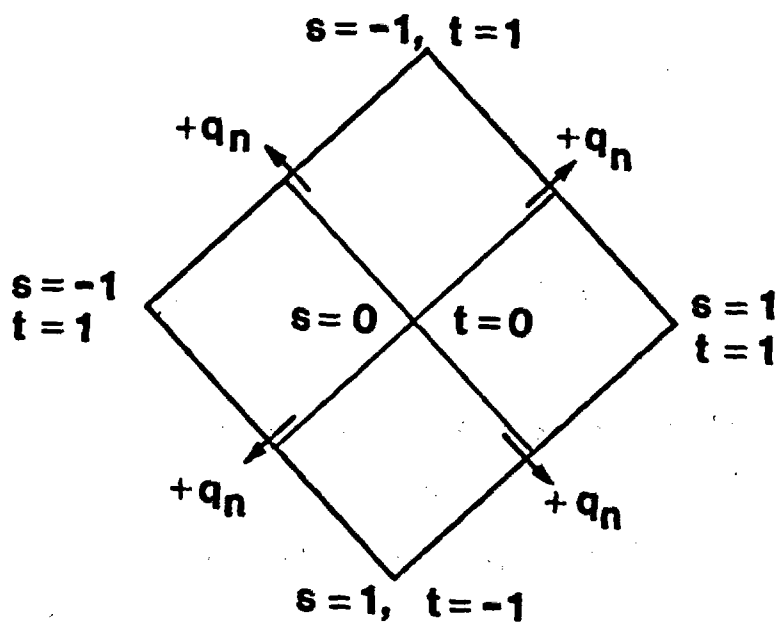
where β is the compressibility, ρ_o is the density at the initial temperature T_o , and $\Delta T = T - T_o$. For mass flux calculations, it is generally true that $g\beta\Delta T \ll 1$, and thus, the water density is assumed to be constant. Using this assumption, the original integral (1) becomes

$$\rho_f \int \Theta^T |J| ds dt \Theta(t) \quad (5)$$

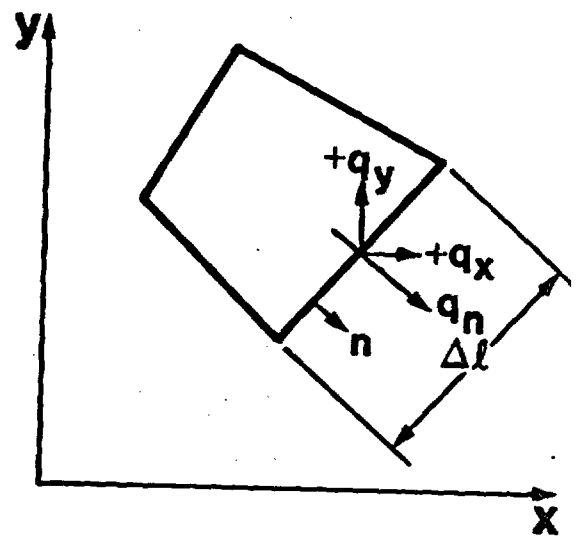
with $\Theta(t)$ being the only time-dependent term. The time-invariant portion of Equation (5) is calculated once per run, along with the geometric shape functions in the FORMKF subroutine. At each time step, the calculated moisture content $\Theta(t)$ is used to evaluate the integral in Equation (5) to solve for the total mass stored. The mass-stored value is then compared to the value at the last time step to compute the change in mass stored.

2.2 Mass Flux Across the Boundary

The exterior sides defining the boundary of the mass-balance area are derived automatically from the list of elements specified by the user. This boundary may define a contiguous region or be made of disjoint parts. Flux across the boundary of an arbitrary region is expressed in terms of the natural coordinates (s,t) for an element; see Figure 1-1a.



1a. Normal Flux
in Natural Coordinates (s,t)



1b. Orthogonal Components
of Total Flux (x, y)

Figure 1-1. Mass-Flux Coordinates

The normalized flux q_n is positive in a direction out of the element, whereas the orthogonal fluxes q_x and q_y are positive up and to the right (see Figure 1-1b). The mass-flux equations based on this sign convention, where n_x and n_y are the x and y components of the unit normal vector n, are derived as follows:

$$q_n = [(q_x n_x + q_y n_y) \Delta \ell] \Delta t = [(q_x \frac{\partial y}{\partial \ell} + q_y \frac{[-\partial x]}{\partial \ell}) \Delta \ell] \Delta t .$$

Therefore,

$$q_n = [(q_x (y_{i+1} - y_i) - q_y (x_{i+1} - x_i))] \Delta t \quad (6)$$

with x_i, y_i and x_{i+1}, y_{i+1} the cartesian coordinates of points i and i+1, respectively, and $\Delta \ell$ is the length of a side dA. If u and v are the horizontal and vertical components of the velocity, then the orthogonal fluxes are given by

$$q_x = \rho_f u_{\text{average}} = \rho_f (u_i + u_{i+1})/2 \quad (7a)$$

and
$$q_y = \rho_f v_{\text{average}} = \rho_f (v_i + v_{i+1})/2. \quad (7b)$$

The total normal mass flux across an element boundary is

$$q_n = 1/2 \rho_f \Delta t [(u_i + u_{i+1})(y_{i+1} - y_i) - (v_i + v_{i+1})(x_{i+1} - x_i)]. \quad (8)$$

3.0 PROGRAM INPUT REQUIREMENTS

The input data required to use the mass-balance option are given below. The format of this section is identical to the one used in the SAGUARO user's manual (Eaton, Gartling, and Larson, 1983). Reference should be made to this manual to completely understand the structure of the input data.

3.1 Mass Command Card

The MASS command requests the computation, at every time step, of a mass balance over a defined region. To allow for an arbitrary region, possibly non-contiguous, the MASS command allows selection of individual grid elements. The selection of elements may be set up by using one or more of the following command cards:

MASS,delimiter type,n1,n2,....,n50.

where

delimiter type is an alphanumeric name indicating how the element arguments are to be interpreted. If delimiter type = SINGLE, each argument is an individual element number. If delimiter type = RANGE, every two arguments are interpreted as a pair, specifying an inclusive series of elements to be included in the mass balance (i.e., MASS,RANGE,5,9,14,18. specifies elements 5,6,7,8,9,14,15,16,17,18).

n1,n2,n3,....,n50 is a list of element numbers indicating which elements are to be included in the mass-balance calculation. A maximum of 50 individual elements or 25 element ranges may be specified on a single MASS command card. There is no restriction on the number of MASS commands or the mixing of MASS cards of different delimiter types in the same input deck.

The MASS command cards must be placed somewhere between the SETUP and FORMKF command cards to be processed correctly. If no MASS command cards are encountered before the FORMKF card, then mass-balance calculations are not performed.

4.0 TEST PROBLEM RESULTS

The objective of these test problems is demonstrating the use of the MASS command in SAGUARO and verifying the accuracy of its algorithm implementation. The test problems presented here include: (1) a simple three-by-three element grid with constant fluid flux in the top and out the bottom of a fully saturated region, (2) a multiple-material, one-dimensional problem in which the boundary mass flux is an imposed condition, and (3) a two-dimensional drainage problem used in benchmarking studies (Hayden, 1984). Mass-balance results (Eaton and Martinez, in preparation) that were calculated in FEMTRAN (Martinez, 1985) for hydrologic flow fields calculated with SAGUARO were used for comparison in Problem 3.

4.1 Problem 1. Three-by-Three Element Grid

This problem consisted of a fully saturated three-by-three element grid with each element side being 1 m in length (Figure 2). A fixed velocity boundary condition of 0.127 m/s was applied at the top and bottom boundaries. The vertical sides are impermeable. This should give a total mass flux of zero. The fluxes were calculated across four individual element sides. The density of water is $1,000 \text{ kg/m}^3$, and the time step is 0.04 s. The vertical mass flux through each horizontal element side should, therefore, be

$$q_y = \rho v A \Delta t = -5.08 \text{ kg/time step.} \quad (9)$$

The values computed with the MASS command compared to this result to better than eight significant places (the displayed accuracy). The fluxes through

the top and bottom sides of each element summed to zero. The horizontal mass flux through the vertical side of each element should also be zero because no driving force is applied. Horizontal fluxes ranging from $1. \times 10^{-10}$ to $1. \times 10^{-14}$ kg/time step were computed. These nonzero horizontal small fluxes resulted from machine roundoff and other numerical inaccuracies. The total residual flux through all the boundary sides over the whole region was computed to be 2.3×10^{-10} kg/time step.

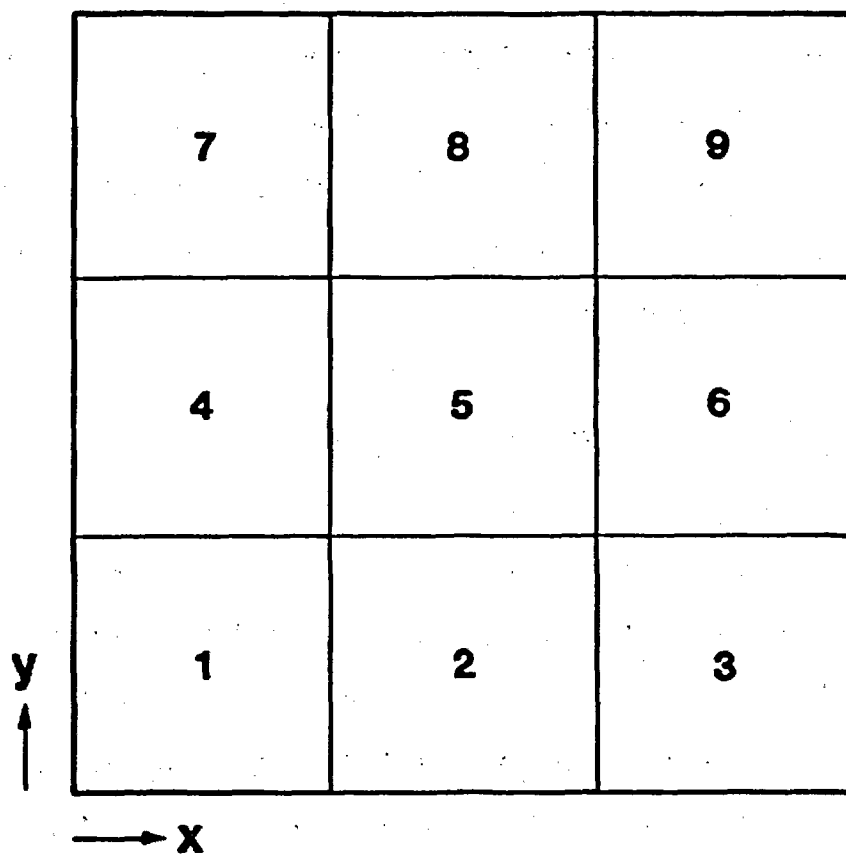


Figure 4-1. Three-by-Three Element Grid for Problem 1

4.2 Problem 2. One-dimensional Infiltration with Multiple Material Strata

This is a simplified one-dimensional model of infiltration in multi-layered tuff (Figure 4-2), using properties given by Eaton (1983). One hundred elements divided into five distinct material strata are used. A constant Darcy velocity influx of 3.17×10^{-8} m/s is applied at the top surface. All other boundaries are held impermeable (i.e., the problem is analogous to filling a bucket containing porous material). Each element is 10 m wide by 1 m deep, varying in height. The water density is 994 kg/m^3 . The time step is 3.15×10^7 s (1 yr). Thus, the mass flux through the top boundary can be calculated to be

$$q = \rho v A \Delta t = 9925.6 \text{ kg/time step.}$$

Computed mass-balance results for every 5 yr are shown in Table 4-1. The calculation of the mass flux at the boundary quickly converges to 9925.6 kg/time step. The difference between the change in mass stored per time step and the boundary mass flux (net gain) indicates the degree of convergence of the hydrological solution at any time step. The normalized net gain (net gain/stored mass * 100) is a percentage-error term that is small for all time steps. Under upon the prescribed boundary conditions and initial moisture distribution, the entire region fills in approximately 73 yr. The total stored mass for a completely saturated grid is solved analytically to be 2.72×10^6 kg. According to Table 4-1, the calculated stored mass value is converging to this value. At the time the region fully saturates, calculations become nonphysical because of the imposed boundary conditions (no flow at bottom, constant infiltration at top).

TABLE 4-1.
Computed Mass
Conservation Values

Time (years)	Stored Mass (kg)	Δ Mass (kg/tstep)	Flux (kg/tstep)	Net Gain (kg)	Normalized Net Gain (%)
5	2060690	10409	-10614	-206	.1
10	2111980	10199	-10260	-61	.00289
15	2162480	10079	-10071	8	.00037
20	2212740	10012	-9935	77	.00348
25	2263020	10042	-9926	116	.00513
30	2313170	10042	-9926	117	.00506
35	2363480	10068	-9926	143	.00605
40	2413860	10069	-9926	144	.00597
45	2463630	9846	-9926	-80	-.00325
50	2510880	8919	-9926	-1007	-.04011
55	2553890	9619	-9926	-307	-.01202
60	2602400	9731	-9926	-194	-.00746
65	2650770	9600	-9926	-326	-.01230
70	2698140	9250	-9926	-676	-.02505

where

- Stored Mass = total mass stored within the region
- Δ Mass = change in the mass stored within the region during the last time step
- Flux = mass flux through all boundary sides during last time step
- Net Gain = Δ mass - flux
- Normalized Net Gain = net gain/stored mass

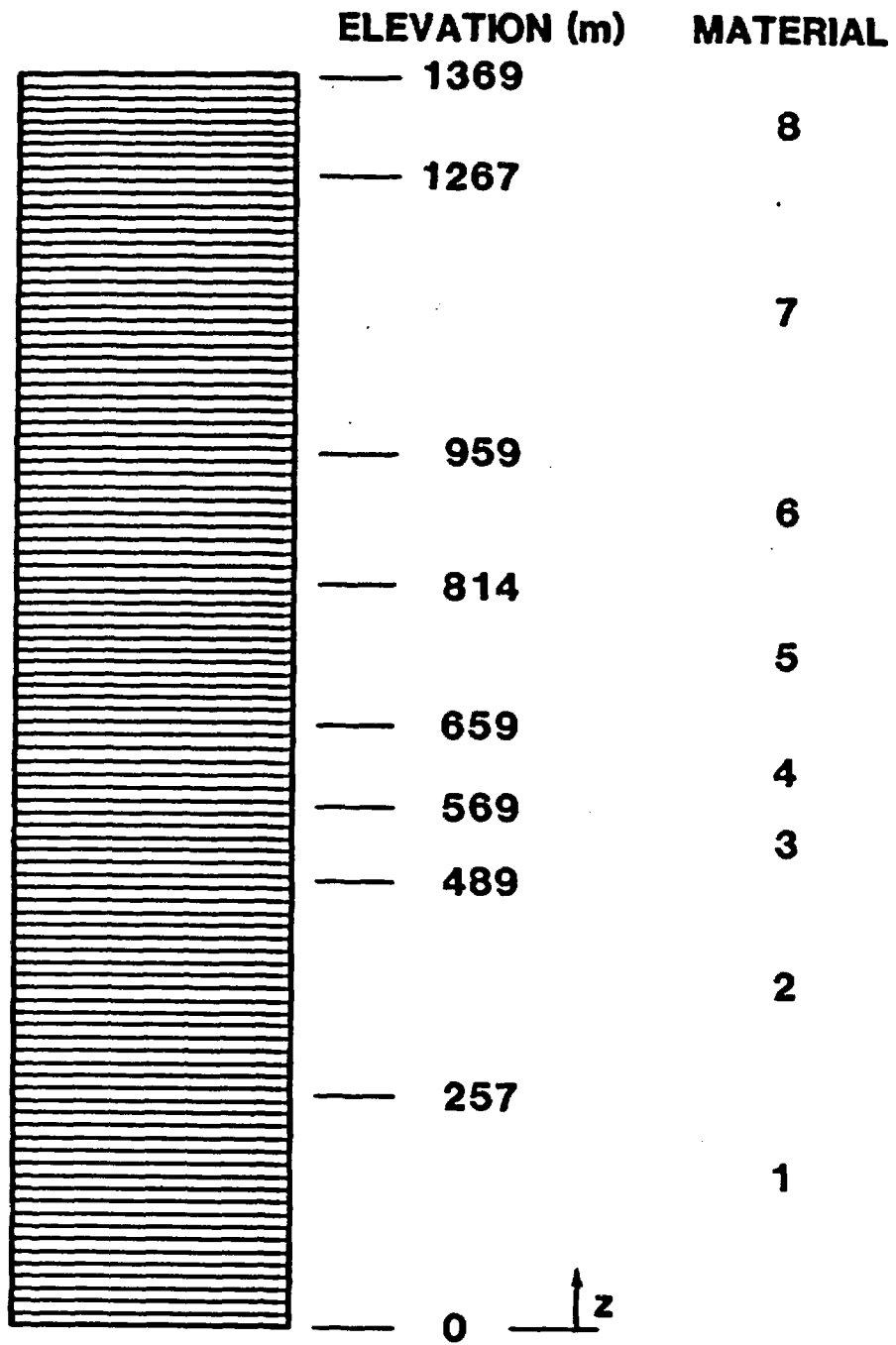


Figure 4-2. Element Grid for One-Dimensional Multi-Strata Problem

4.3 Problem 3. Two-Dimensional Drainage Problem

This drainage problem was first posed by Pickens et al, 1979, and was used extensively in the NNWSI COVE benchmarking series (Hayden, 1984; Eaton and Martinez, in preparation). A mass-balance calculation was made by linking the hydrologic solution of SAGUARO to the solute transport code FEMTRAN (Eaton, 1983) and was used as the basis of comparison. A finite-element grid of 221 elements was used for these solutions (see Figure 4-3) in which the initial stored mass is 7,500 g. Initial and boundary conditions are identified in Figure 4-4. The first 4 hr of this transient solution were compared. Mass-balance values computed by FEMTRAN are shown in Table 4-2. Some numerical error is always introduced when coupling results of SAGUARO to FEMTRAN because of limits that format constraints place on accuracy. The mass balances that SAGUARO calculated with the MASS command are shown in Table 4-3. The net gains of both sets of mass balances are compared graphically in Figure 4-5. A net mass gain of zero implies perfect mass balance. The results of SAGUARO compare favorably with the results of FEMTRAN.

TABLE 4-2
FEMTRAN Mass Balance

Time (min)	Flux (g/tstep)	Δ Mass (g/tstep)	Net Gain (g)	Normalized Net Gain (%)
2.7	-5.7	-9.6	-3.9	0.052
12.	-30.3	-31.3	-1.0	0.013
30.	-67.3	-62.6	4.7	0.063
60.	-110.3	-97.2	13.1	0.175
120.	-138.9	-123.5	15.4	0.205
180.	-111.5	-103.7	7.8	0.104
240.	-94.6	-84.0	10.6	0.141

TABLE 4-3
SAGUARO Mass Balance

Time (min)	Flux (g/tstep)	Δ Mass (g/tstep)	Net Gain (g)	Normalized Net Gain (%)
2.6	-5.9	-7.2	-1.3	-0.017
13.	-30.2	-29.9	0.3	0.004
30.	-65.9	-62.1	3.8	0.051
60.	-108.7	-100.2	8.5	0.113
120.	-137.4	-126.4	11.0	0.147
180.	-110.6	-102.7	7.9	0.105
240.	-93.0	-86.9	6.1	0.081

where

- Stored Mass = total mass stored within the region
- Δ Mass = change in the mass stored within the region during the last time step
- Flux = mass flux through all boundary sides during last time step
- Net Gain = Δ mass - flux
- Normalized Net Gain = net gain/stored mass

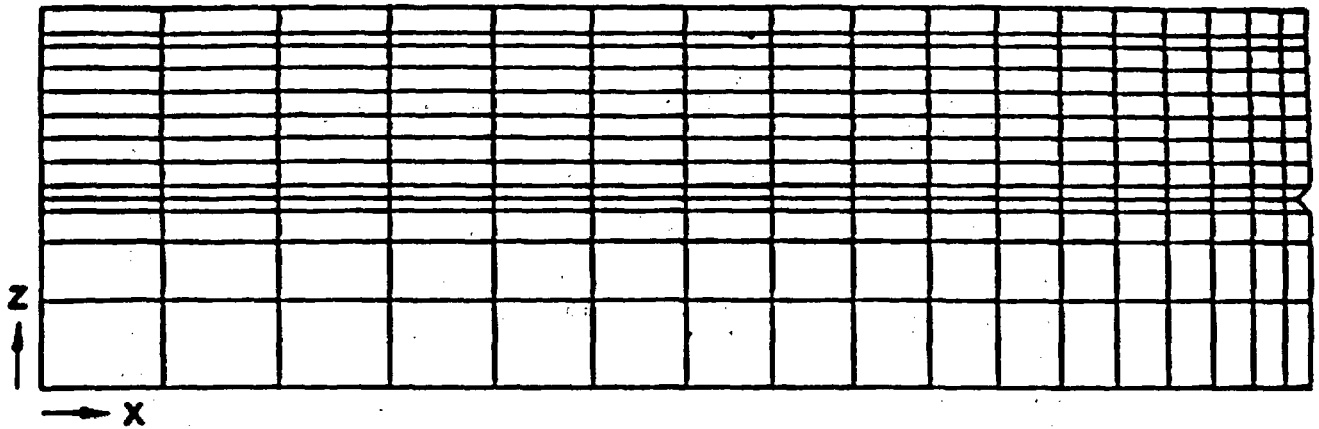


Figure 4-3. Element Grid for Tile Drainage Problem (221 Elements)

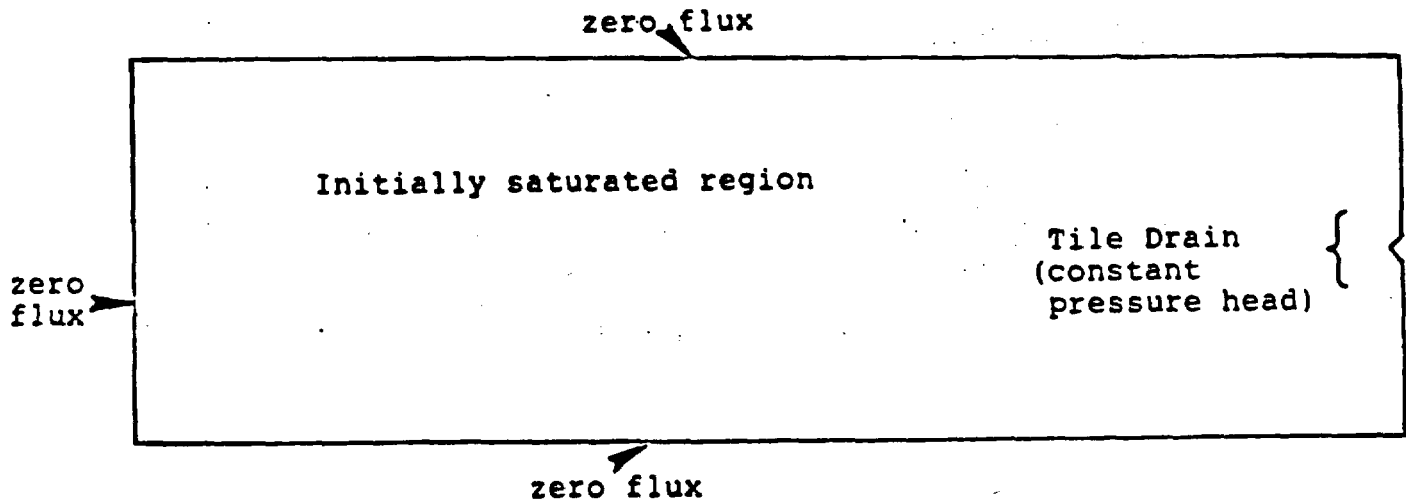


Figure 4-4. Boundary and Initial Conditions for Tile Drainage Problem.

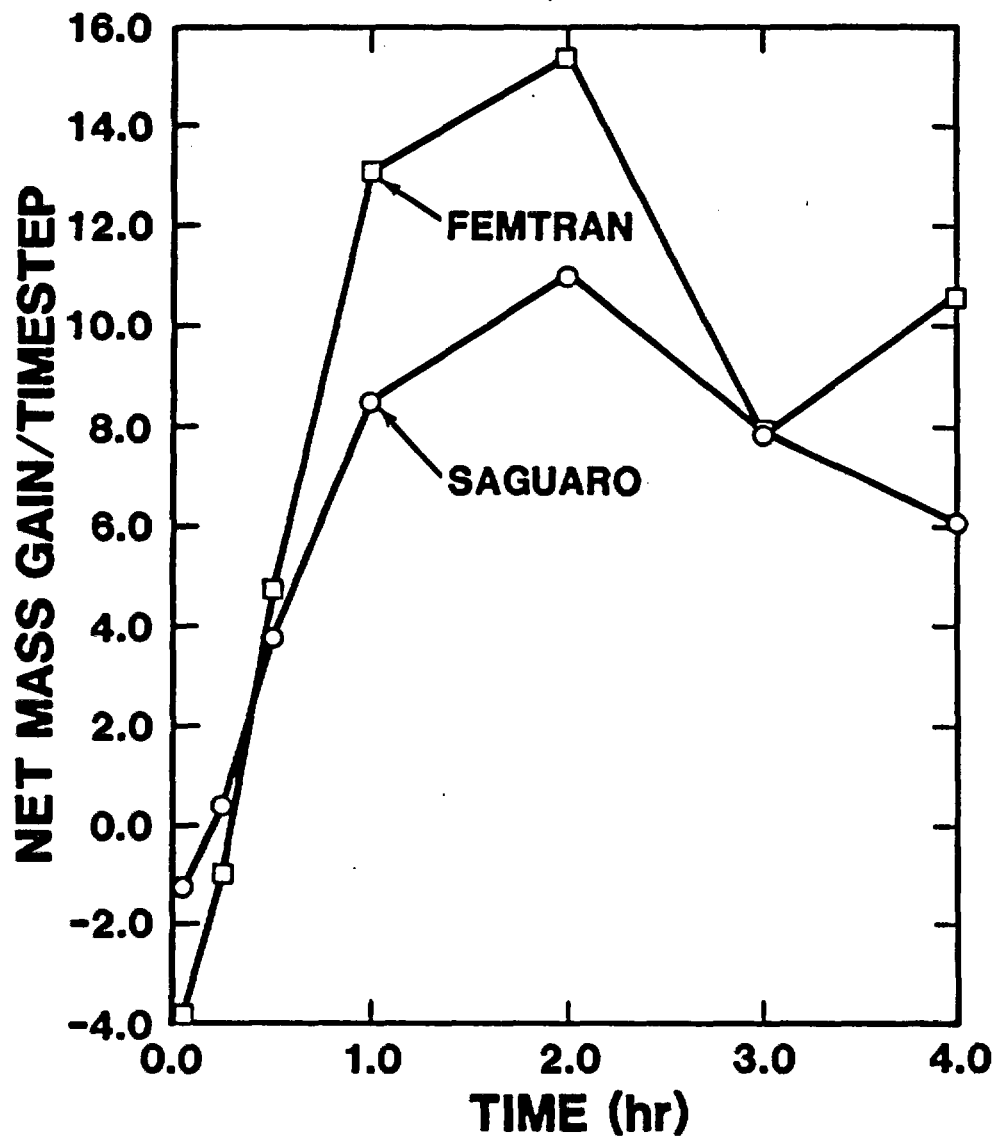


Figure 4-5. Mass Balance as a Function of Time for Problem 3

5.0 CONCLUSIONS

The mass-balance routine described in this report has been developed to assess the accuracy of results calculated by the finite-element code SAGUARO. The computer time required to execute the mass-balance calculations is minimal, and the input data requirements are straightforward.

In Problem 1, the implementation of the mass-balance calculations in a saturated two-dimensional flow field was verified with an analytical solution. The mass flux across all interior and exterior element sides and the total mass stored were correctly calculated by the mass-balance subroutine.

Problem 2 was used to verify the mass-balance calculations in SAGUARO for time-dependent problems with multiple material strata. The actual mass-balance values for the run were known a priori and compared to the mass balances calculated by the new subroutine.

Results of a more complex sample calculation, Problem 3, show that the net mass balances calculated with the new subroutine in SAGUARO are more accurate than those calculated by FEMTRAN. In general, the mass balances calculated in SAGUARO are closer to zero than the corresponding balances calculated by FEMTRAN. The results imply that the mass balances calculated with the new subroutine in SAGUARO are better than mass balances obtained by coupling SAGUARO and FEMTRAN.

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