Chapter 5

MODEL CALIBRATION AND RESULTS

Calibration Strategy

A quasi three-dimensional finite-difference ground-water flow model was designed and calibrated to: 1) quantify the hydrologic parameters representing the hydrogeologic units of the study area, 2) establish the role of the South Coast Fault Zone and its influence on the migration of seawater into the basins, 3) provide the overall hydrologic budget of the basins, 4) determine the impact of river recharge on the flow regime of the Rio Cobre and Rio Minho-Milk river basins, and 5) produce a map of the potentiometric surface in the White Limestone and alluvial aquifers. Calibration of the model is a process of updating selected model parameters based on the results of previous simulations to derive a close match between the observed steady-state water levels and calculated hydraulic heads in the model. A steady-state simulation of hydraulic head conditions for the water year 1998 was used to calibrate the model. Steady-state conditions imply that the system is in equilibrium, such that total inflow is equal to total outflow.

A calibration target of 8 m was set as the accepted margin of difference between calibrated and observed heads for each well observation point used to calibrate the model. The model was calibrated using initial *trial and error* adjustments to selected input parameters followed by statistical linear regression analysis performed by the model. Adjustments were made to: 1) recharge, 2), conductance values at the general-head boundary, 3) the hydraulic conductivity field, 4) the width of the barrier along the South Coast fault, 5) the Kx/Kz ratios, and 6) streambed vertical hydraulic conductivity until an acceptable match between calculated and observed hydraulic heads was achieved. A map of the distribution of hydraulic head observation points used to calibrate the model is presented in Figure 5.1. There are three notable conditions or strategies that were crucial to the final development and calibration of the model: 1) the simulation of a general-head condition along the northern boundary, 2) the successive adjustment of hydraulic conductivity to the White Limestone aquifer, especially in the lower Rio Minho-Milk River basin, and 3) the simulation of a horizontal-flow barrier along the South Coast fault.

Recharge rates were assigned to vary in regions by weights based on steepness of slope. During model calibration, applied ground-water recharge was adjusted according to topographic features. In areas within the irrigated plains, the range of values was from 110 mm/yr to 250 mm/yr. Recharge over the karst highland plateaus ranged from 85 mm/yr to 280 mm/yr. In upland regions, the range was from 150 mm/yr to a maximum of 385 mm/yr (Figure 5.2). Recharge rates for the upland regions are assumed far greater than those for: the highland plateaus, lower permeability materials (crystalline areas) of the upper Rio Minho-Milk River basin, or areas where agricultural drainage may limit infiltration in the coastal plains (Springer and Bair, 1992).

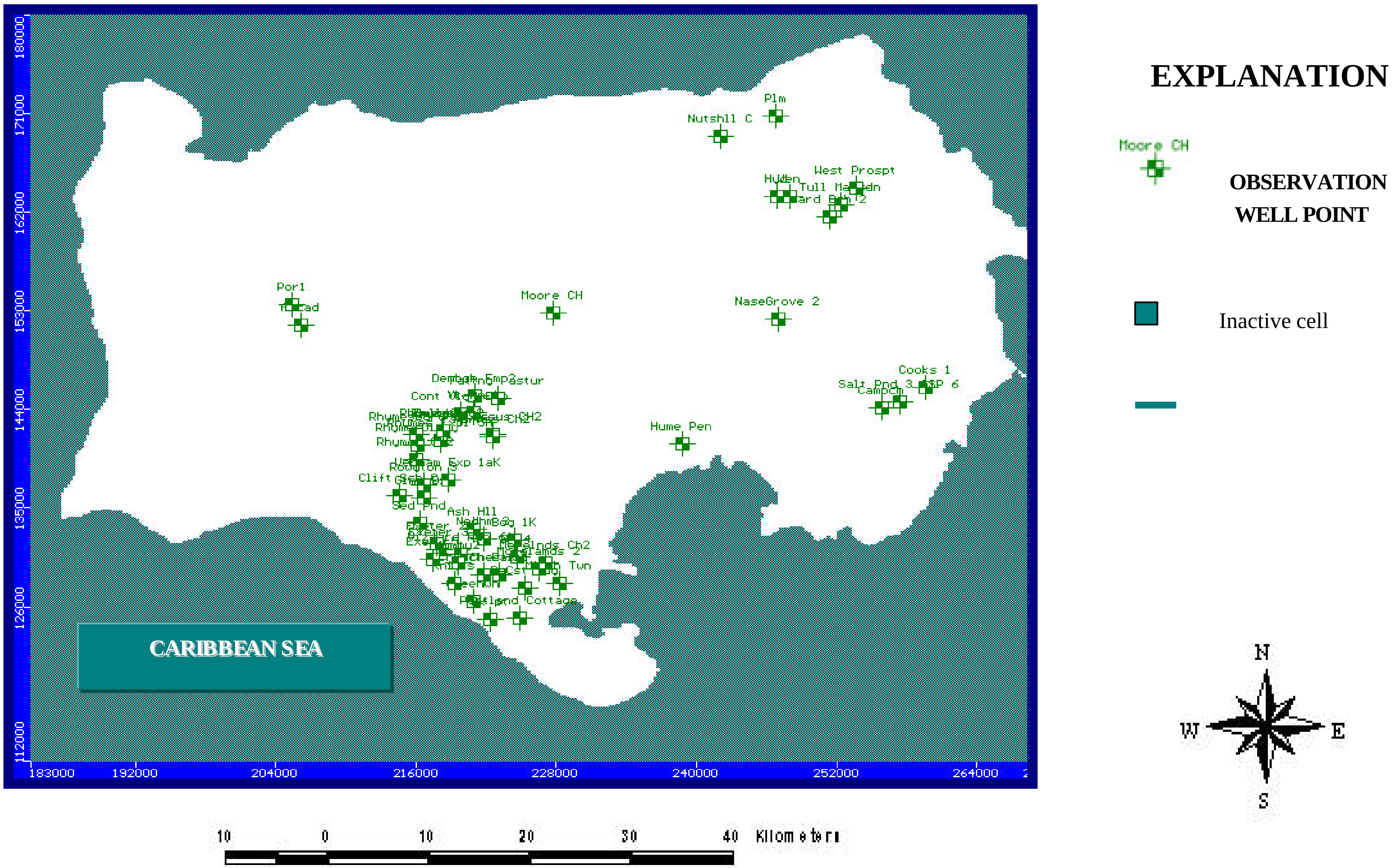

Figure 5.1 Distribution of observation wells in the Rio Cobre and Rio Minho-Milk River Basins used to calibrate the model.

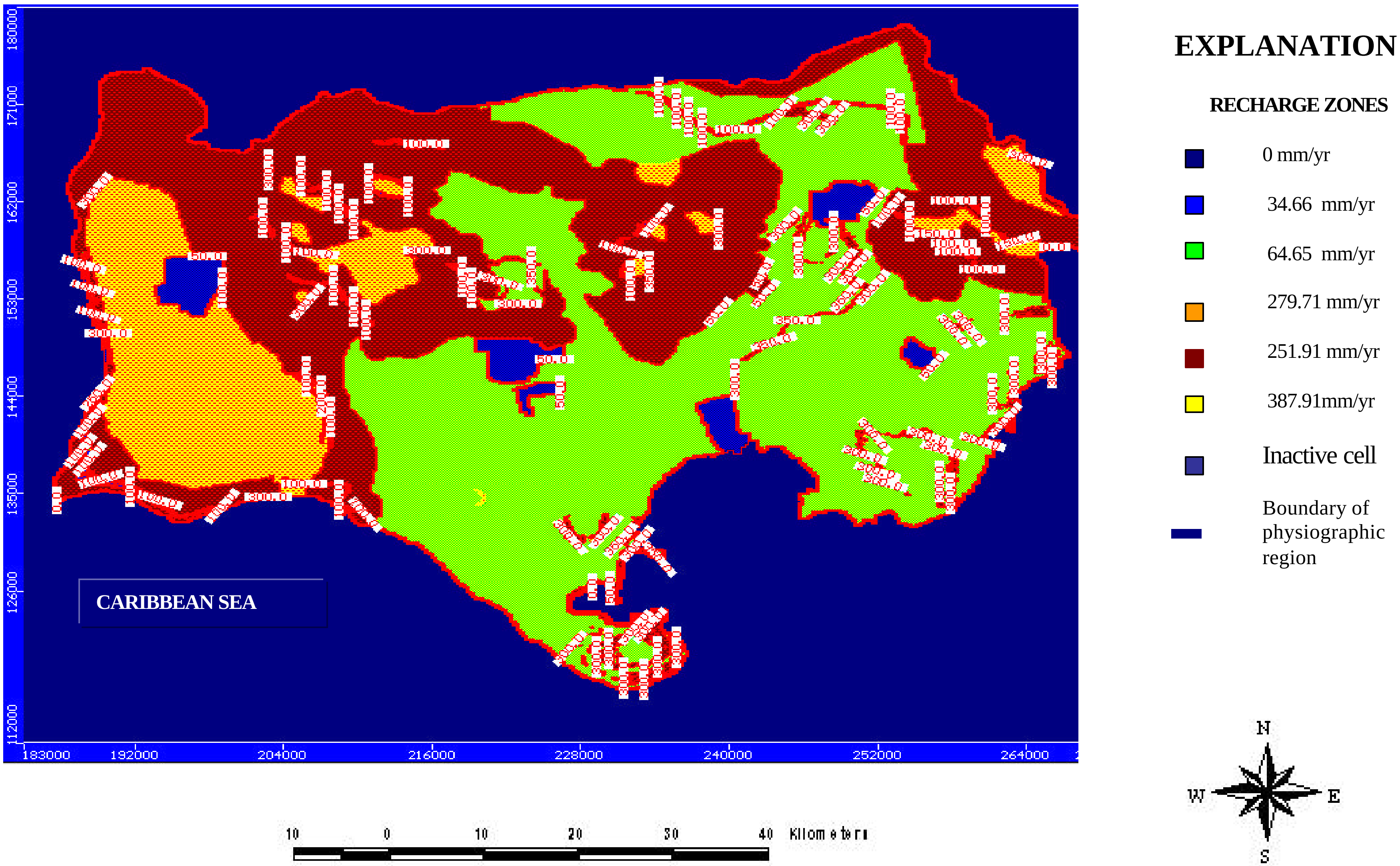

Figure 5.2. Map of calibrated recharge zones in model layer 1

Initial simulations were conducted with no-flow conditions along the upper boundary and later changed to a general-head boundary. No-flow was initially used to determine the appropriate hydraulic conductivity and recharge values required to limit unrealistically large volumes of inflow across this boundary. The model would not calibrate with no-flow conditions imposed at the boundary. The assignment of constant-head cells along the upper boundary was not effective in calibrating the model. Model insensitivity to theses changes may have been related to the location of the upper boundary that is situated below a topographic divide at approximately 5 - 10 kilometers from the anticlinal axis of the Central Inlier, the island's main watershed or the hydraulic head values assigned at the boundary, based on the extrapolation of depth to water level. The assignment of a general-head boundary was assumed appropriate to provide stability to the model allowing it to calculate the distribution of hydraulic heads in the basin and also provide a way to estimate the upland subsurface inflow that may be occurring through the upper boundary. Specifying a hydraulic conductance value proportional to hydraulic conductivity between the aquifer and the boundary controls inflow and simulated heads along the boundary.

The most effective calibration technique for the adjustment of the hydraulic conductivity field in the model was to initially delineate fewer conductivity zones and then gradually increase the number of zones based on the geology and permeability of the hydrogeologic unit in the region. The geometric mean was then used for averaging horizontal hydraulic conductivity in fifteen zones, since the pattern of heterogeneity appeared to be randomly distributed. The adjustment procedure involved successive changes to horizontal hydraulic conductivity values (Kx) conducted from the upper boundary to lower boundary of the model. Karstic regions in the lower Rio Minho-Milk River basin and alluvial fills like the alluvium graben were assumed to be more permeable than areas of crystalline rocks outcropping mainly in the upper Rio Minho-Milk River basin.

Fifteen hydraulic conductivity zones were originally assigned to the area based on the variation in geology (Table 13). One of the fifteen hydraulic conductivity zones simulated earlier in the model calibration included a zone of cells representing the South Coast fault that transects the lower Rio Minho-Milk River basin (Figure 2.8). A high, average hydraulic conductivity value of 222 m^3/d was assigned in both directions of the fault. Initially, the barrier width of the fault was assumed to be 1.0 m instead of 0.5 m. Flow in the vertical direction was not inhibited, but flow parallel to the fault was inhibited, resulting in a steep hydraulic gradient near the coastline. This caused difficulty in obtaining an agreeable match between the calculated and observed heads in the lower Rio Minho-Milk River basin. To simulate the potential conditions along the fault and how the fault may impact the potentiometric surface of the Rio Cobre and Rio Minho-Milk river basins, the Horizontal-Flow Barrier Package (HFB) (Hsieh and Freckleton, 1993) was used to simulate the cells along the fault.

A horizontal to vertical hydraulic conductivity (Kx/Kz) ratio of between 1 and 10 is usually assumed for porous media in most hydrologic modeling studies. An initial Kx/Kz ratio of 10:1 was also assumed for the aquifers in this modeling study. The ratios

Table 13. Estimated versus calibrated hydraulic conductivity (K) values used in model analysis of the Rio Cobre and Rio Minho-Milk river basins.

Aquifer	**Zone**	**Estimated Hydraulic Conductivity K_x (m/d)**	**Estimated Vertical Hydraulic Conductivity Ky (m/d)**	**Calibrated Hydraulic Conductivity K_x (m/d)**	**Calibrated Vertical Hydraulic Conductivity Ky (m/d)**
White Limestone	1	135	26	70	7
	2	135	26	70	7
	3	135	26	60	3
	4	165	32	33	7
	5	780	78	482	120
	6	25	12	25	12
	7	25	12	40	10
	8	222	222	N/A	N/A
	9	40	8	40	4
	10	40	8	30	8
Alluvium					
	11	25	12	35	7
	12	25	12	50	10
	13	780	78	100	20
	14	30	15	70	14
	15	165	32	30	6

were continually adjusted during calibration according to the geology and permeability in each hydraulic conductivity zone. The model was calibrated with a ratio of 20:1 notably in two areas: 1) in the crystalline upland rocks in the upper Rio Minho-Milk River basin (zone 3) and zone 15, bordered by the coastline and the South Coast fault (Figures 5.3 - 5.4). It is inferred that the high Kx/Kz ratio in zone 15 is related to the upthrow of rocks of lower permeability along the South Coast Fault. The areas observed to have the lowest Kx/Kz ratio 4:1 were the ancient Tertiary carbonate platform underlying the Recent alluvial aquifer in the lower Rio Minho-Milk River basin and zone 12, the White Limestone-alluvium contact in the lower Rio Cobre basin. These low ratios reflect the more nearly isotropic nature of these deposits.

No data on streambed vertical hydraulic conductivity were available. Therefore, the adjustment of streambed vertical hydraulic conductivity was constrained to the range of values obtained from laboratory tests or other ground-water flow reports (Rosenshein et al., 1968; Vogel and Reif, 1993). Although streambed vertical hydraulic conductivity may vary locally, the same initial value was assigned to all hydrogeologic units because of lack of data. Calibration of the streambed hydraulic conductivity was accomplished by adjusting the initial value of streambed hydraulic conductivity in the same manner for all stream reaches overlying the same hydrogeologic unit. An initial value of 0.083445 m/d was assumed for streambed sediments in this study, based on values reported by Vogel and Reif (1993) for streambed vertical hydraulic conductivity in similar sediments (clay, volcanics, and minor limestone).

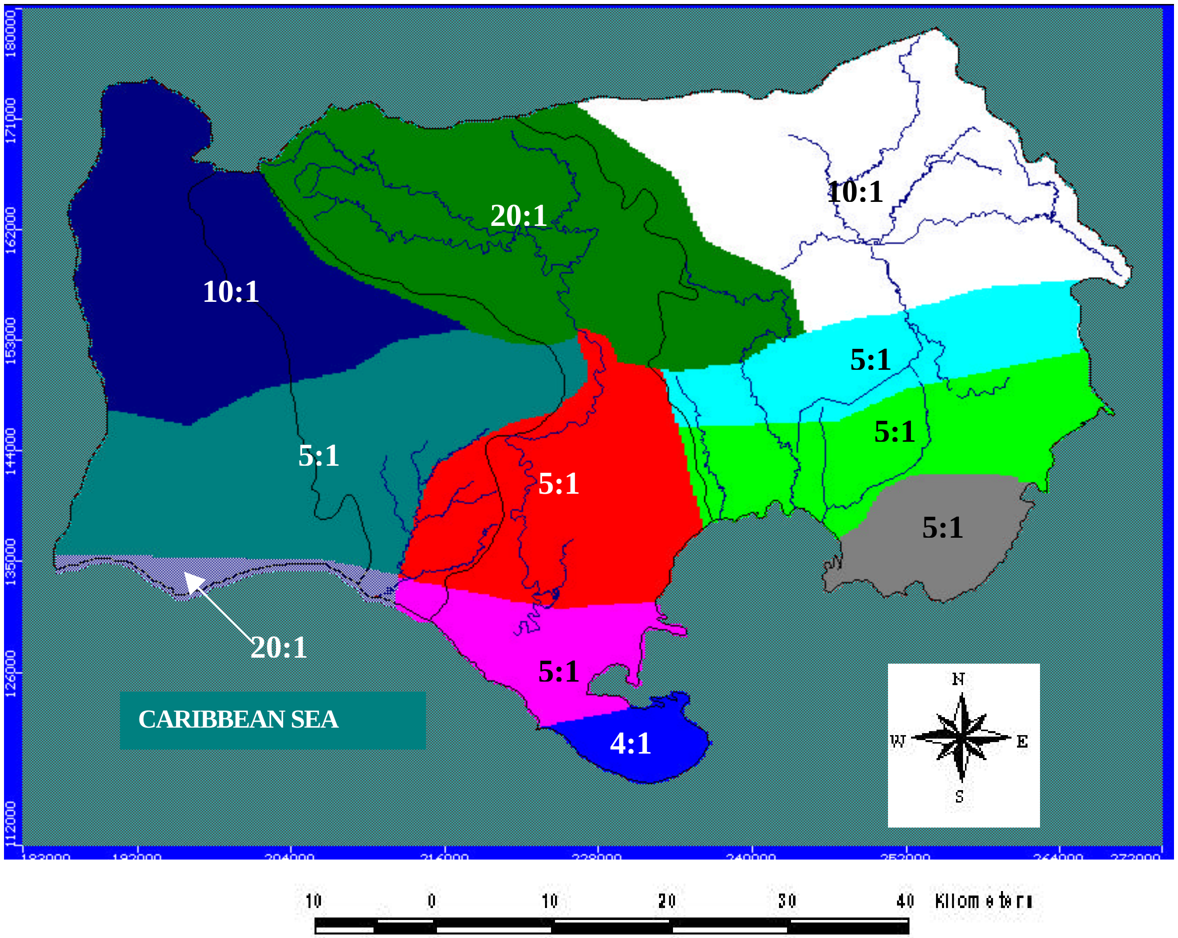

Figure 5.3 Map of calibrated hydraulic conductivities and of the distribution of Kx/Kz ratios in model layer 1- alluvial aquifer.

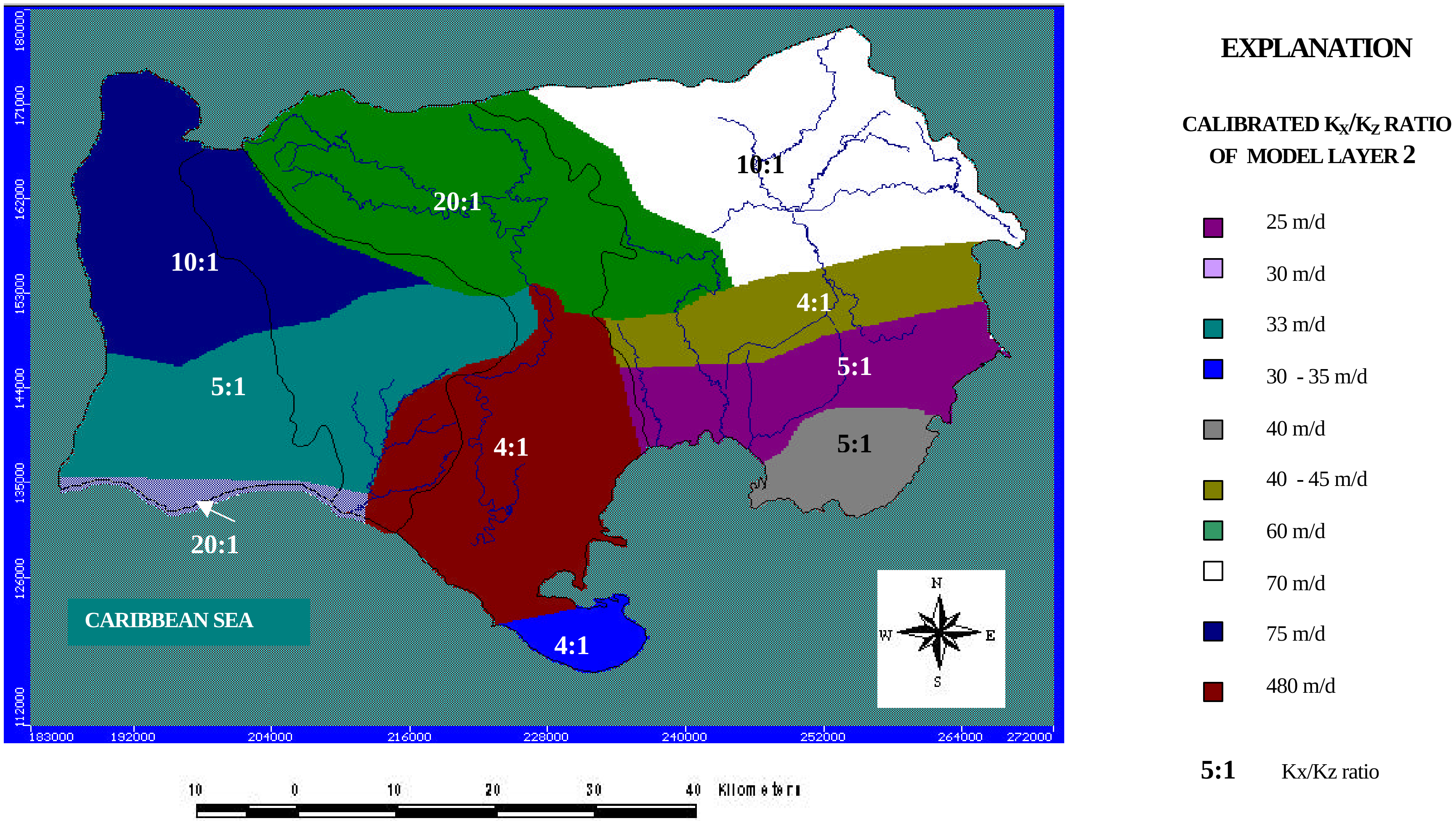

Figure 5.4 Map of calibrated hydraulic conductivity zones and the distribution of K_x/K_z ratios in model layer 2 – White Limestone aquifer.

Calibration Criteria

The criteria used to determine an acceptable match between calculated and measured hydraulic heads are subjective, despite the goal of minimizing the difference between calculated and measured heads. The calibration criteria involved:

1) A fairly good visual comparison between the measured and simulated heads and potentiometric surfaces.
2) A root-mean square error between measured and simulating heads of less than 8.00 m (figure 5.5).
3) Overall significant improvement in the match between calibrated versus observed heads from the assignment of the HFB along the South Coast fault and the final adjustment of the hydraulic conductivity in the old carbonate platform in the lower Rio Minho-Milk River basin.
4) Confirmation of the role of the South Coast fault as a low permeable conduit for ground-water flow parallel to the fault and the migration of seawater into the lower Rio Minho-Milk River basin (Mullings and Howard, 1993).

The map of the calibrated potentiometric surface shown in Figure 5.6 bears a fairly close resemblance to the map of the generalized water table in figure 3.12.

Root Mean Squared Error

Statistical analysis is performed by MODFLOW after manual *trial-and-error* adjustment to selected input parameters. It involves regression analysis and the

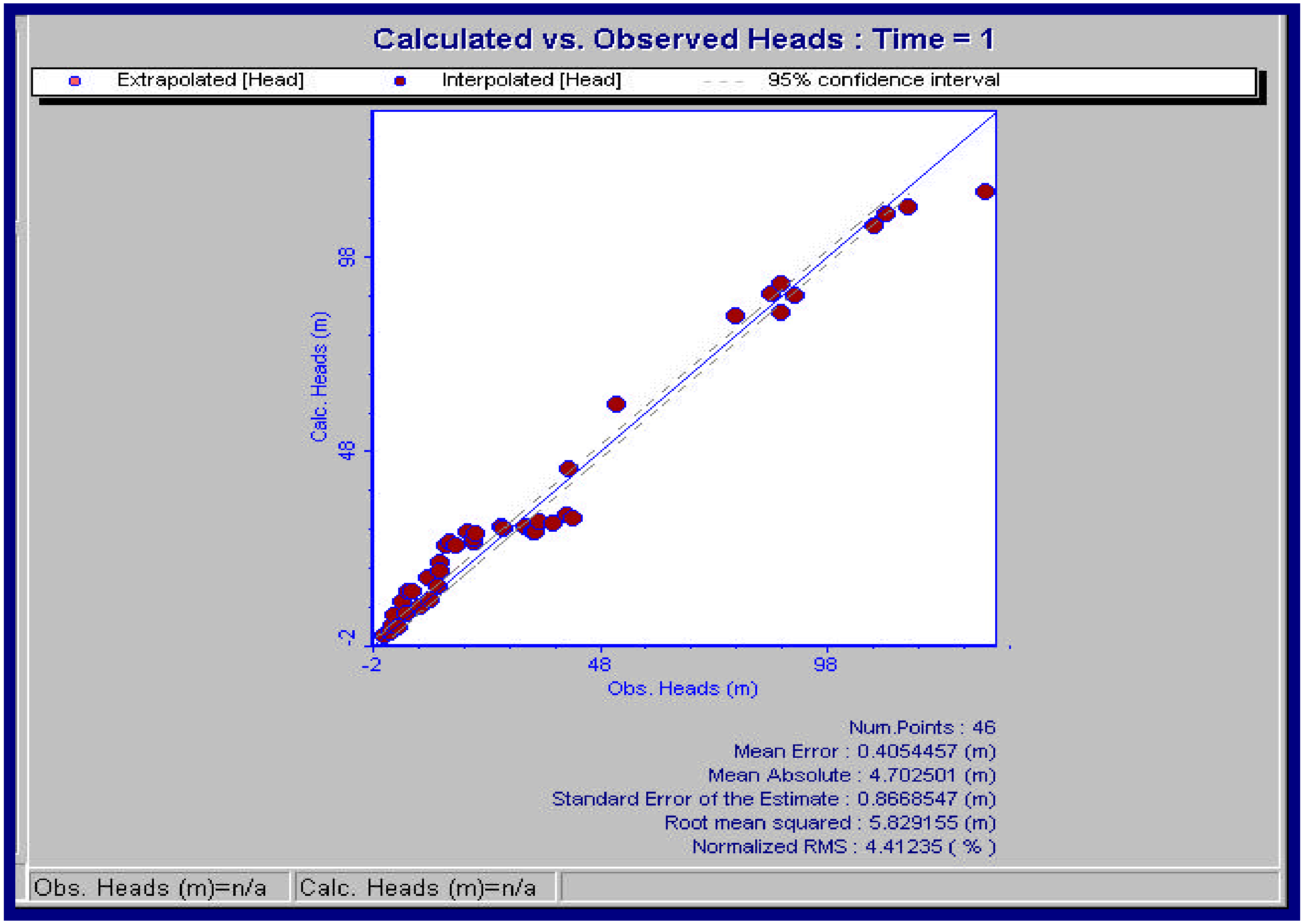

Figure 5.5 Calibration plot of calculated versus observed heads in the White Limestone aquifer and alluvial aquifers of the Rio Cobre and Rio Minho-Milk river basins. The results of the simulation are shown above. Heads were plotted as shown. Confidence intervals for the linear regression analysis are also shown.

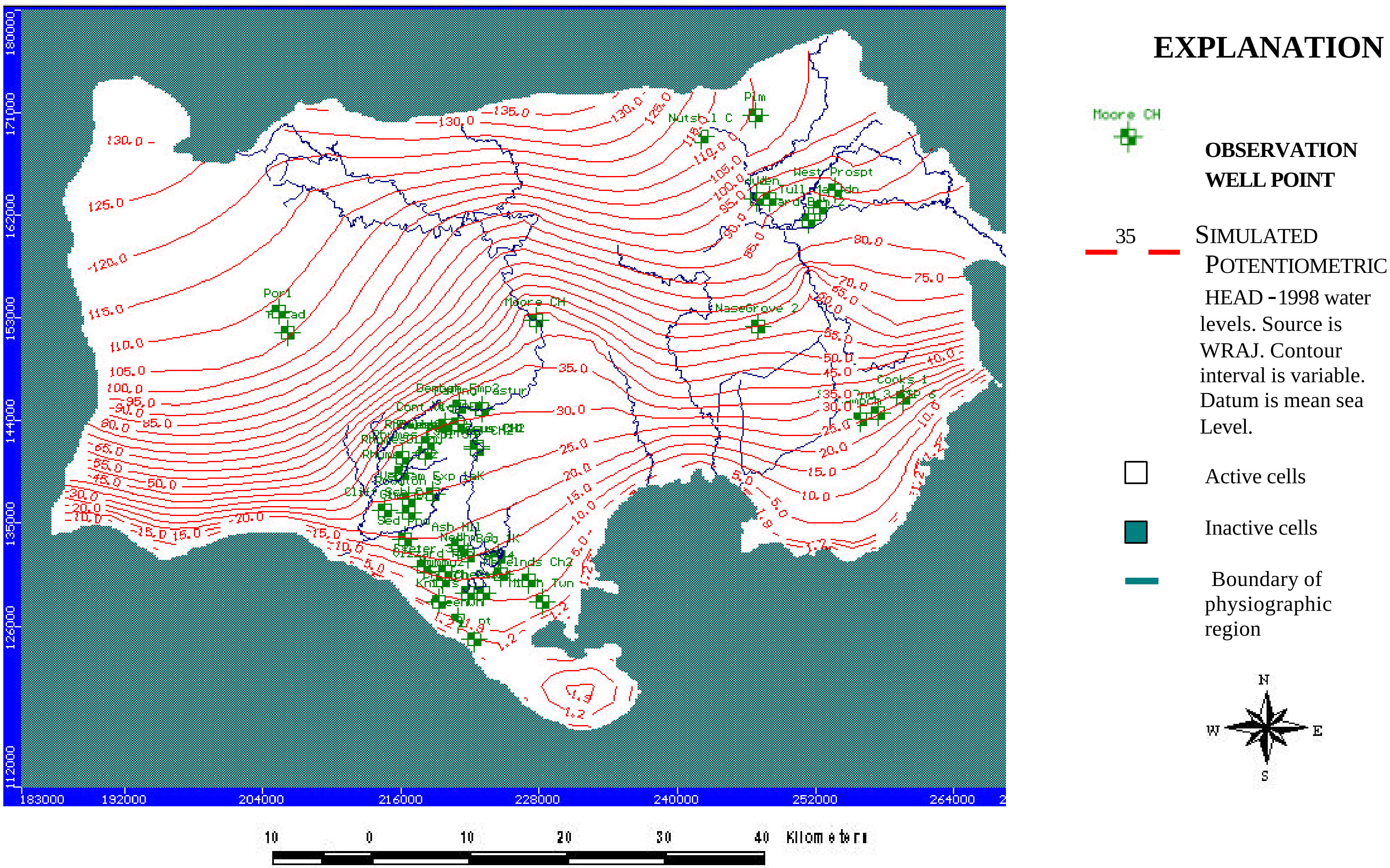

Figure 5.6 Simulated water table surface of the White Limestone aquifer of the Rio Cobre and Rio Minho-Milk river basins, Jamaica.

calculation of the root mean squared error (RMSE). The root mean squared error, or the standard deviation, is the average of the squared differences in measured and simulated heads. It is also a measure of the error in the simulated head over the entire modeled area, used as the overall criterion for determining whether the hydraulic variable considered should be increased or decreased. The RMSE is calculated by the following equation:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{n}\left(h_m - h_s\right)^{0.5}} \qquad (13)$$

where,

N is the total number of hydraulic head observations in the study area

h_m is the observed hydraulic head

h_s is the calculated hydraulic head

If the RMSE decreased, then the adjustments to the input data were retained. In addition to the RMSE, the percentage difference between measured and simulated heads was evaluated. If the percentage difference decreased, then adjustments to the input data were retained. The model was considered calibrated when the following criteria were met:

1) Simulated flow directions agreed with those represented in the water table map constructed from the static water level measurements of 46 wells.
2) The calculated heads reasonably matched measured or inferred heads (Figure 5.5-5.7).

3) Visual inspection of the areal distribution of the residuals or differences between heads interpolated from the water level map and simulated heads indicated no consistent pattern of positive and negative high or low values.
4) A distribution of aquifer and streambed hydraulic conductivity was maintained within the range of values obtained from published values for laboratory tests, reports, and from some specific-capacity tests done in the Rio Cobre and Rio Minho-Milk river basins.

Changes in simulation results were compared to corresponding changes in model parameters and are based on RMSE values. However, a major improvement in model calibration and development was observed when the South Coast fault was simulated as a low permeable feature. The results from the analysis are used as a tool to understand the limitations of the data upon which the model is based.

Simulation of the South Coast Fault

The Horizontal-Flow Barrier Package (HFB) (Hsieh and Freckleton, 1993) was used to simulate the vertical, low permeable South Coast Fault Zone (SCFZ) in the lower region of the Rio Minho Milk River Basin. In the finite-difference grid, the feature is treated as a horizontal, but low permeable flow barrier in both model layers (Figure 5.8). The HFB Package simulates thin vertical, low-permeability geologic features that impede