3/17/92

Dynamic Coupling - A New Tool for Three-Dimensional Flow and Transport Simulations

Andreas Haug[1], Gerald E. Grisak[1], and Frederick G. Wolf[2]

[1]INTERA Inc.
Austin, Texas

[2]ATOCHEM North America
Tacoma, Washington

ABSTRACT

Simulating flow and transport in layered geologic media comprising aquifers and aquitards still represents a challenge to current finite-difference modeling techniques. In aquifers, the flow direction is usually horizontal and accurate simulation requires a sufficiently fine horizontal discretization. In aquitards, the flow direction is often vertical which requires grid refinement in the vertical direction. In such a situation, three-dimensional grids typically require tens of thousands of grid blocks. To address such problems, the ground-water simulator SWIFT II was enhanced to include a dynamic coupling option. When using this technique, the aquifers are discretized into normal finite-difference grids. However, the aquitards are discretized into columns of one-dimensional vertical subgrids, which are condensed from the main solution matrix. Dynamic coupling reduces the matrix of a full aquifer-aquitard system to the order and band width of the individual aquifer matrices, resulting in a significant reduction of memory requirements and execution time.

Dynamic coupling was successfully applied in the context of developing and optimizing the aquifer remediation plan for a chemical-plant site in Tacoma, Washington. Past production of an arsenic-based herbicide has resulted in arsenic contamination of the groundwater beneath the plant. A remediation plan was developed to provide a longterm solution to the ground-water contamination. The enhanced version of SWIFT II was used to simulate three-dimensional ground-water flow and arsenic transport during and subsequent to the aquifer remediation.

INTRODUCTION

Traditional finite-difference formulations transform the flow and transport equations into matrix equations. Most of the computer memory requirements and run-time demands are associated with storing and processing these matrices. Experience and theoretical studies have shown that memory requirements and computing time per time-step increase dramatically with the refinement of three-dimensional grids. Price and Coats (1973) have demonstrated that, using direct-solution algorithms with either standard ordering or more sophisticated ordering schemes for Gaussian elimination, the memory requirement can be calculated as follows:

$$M = k_m n_x (n_y n_z)^2 \qquad (1)$$

where n_x, n_y, n_z = dimensions of the finite difference grid with $n_x \geq n_y \geq n_z$

k_m = ordering scheme specific constant ($k_m = 1$ for standard ordering).

Standard ordering schemes number the nodes of a three-dimensional grid first along the shortest direction (z direction), then in the next shortest direction (y direction), and finally in the longest direction (x direction). The maximum band width of the matrix is then $n_x n_y$. Thus, the required memory increases with the square of the band width of the matrix.

Price and Coats (1973) have further demonstrated that the computing time (work) increases with the cubed product of the two smaller grid dimensions:

$$W = k_w n_x (n_y n_z)^3 \qquad (2)$$

where n_x, n_y, n_z = dimensions of the finite difference grid with $n_x \geq n_y \geq n_z$.

k_w = ordering scheme specific constant ($k_w = 1$ for standard ordering).

Thus, the computing time increases with the cube of the band width of the matrix.

Equations (1) and (2) imply that both M and W are most sensitive to increasing or decreasing the number of grid blocks along the shortest directions (i.e., y and z direction). In many applications, the z direction corresponds to the vertical direction of the model domain. Therefore, refining the model grid in the vertical direction often results in more than proportional increases of M and W. On the other hand, the largest gains are obtained from reducing the number of grid blocks along the vertical direction.

DYNAMIC COUPLING

To address this problem, the finite-difference flow and transport code SWIFT II (Reeves et al., 1986a, 1986b) was enhanced to include a dynamic coupling option. Dynamic coupling was developed for applications where, in parts of the model domain (e.g., in aquitards), the direction of flow is primarily vertical. Dynamic coupling specifically exploits the fact that, in such cases, the horizontal flow component in aquitards is negligible. When using this technique, each aquitard is discretized into columns of vertical subgrids ("legs") which, in the absence of lateral coupling, become one-dimensional. These legs correspond to tridiagonal submatrices. They are solved separately from the main matrix using preprocessing, thereby introducing simple source terms into the main matrix. The remaining parts of the model domain (e.g., the aquifers) are discretized in a traditional manner into two- or three-dimensional finite-difference grids, and constitute the main matrix. Upon completion of the main matrix solution, the source terms (from the legs) are evaluated explicitly and the global solution is swept into the aquitards. Thus, dynamic coupling reduces the matrix of the full aquifer-aquitard system (main matrix) to the order and band width of the individual aquifer matrices. Frequently, the latter are only two-dimensional, resulting in a significant reduction in memory requirements and computing times.

As explained above, dynamic coupling condenses the aquitards from the main solution matrix. This condensation essentially introduces a cross-aquitard coupling between the aquifer grid blocks lying immediately above and below the aquitard. However, in reality an aquitard tends to insulate neighboring aquifers because aquitard equilibration times are much larger than the corresponding times in aquifers. In most model applications, time-step lengths are selected based on the relatively fast processes in the aquifers. Therefore, over a given time step, the direct coupling between aquifers may be neglected. Consequently, the submatrix of each aquifer may be solved separately, resulting in an additional reduction in both the memory requirements and the computing time.

A simple example may serve to illustrate the benefits of dynamic coupling. Figure 1 shows a traditional finite-different grid with $30 \times 20 \times 12 = 7200$ grid blocks representing two aquifers separated by an aquitard. The equivalent discretization based on dynamic coupling is shown in Figure 2. Using equations (1) and (2), the memory requirements and the computing times of the dynamic coupling model were calculated to be lower by factors of 144 and 571, respectively, than the corresponding values using standard discretization. This example demonstrates that dynamic coupling makes feasible applications which are almost impossible using standard discretization.

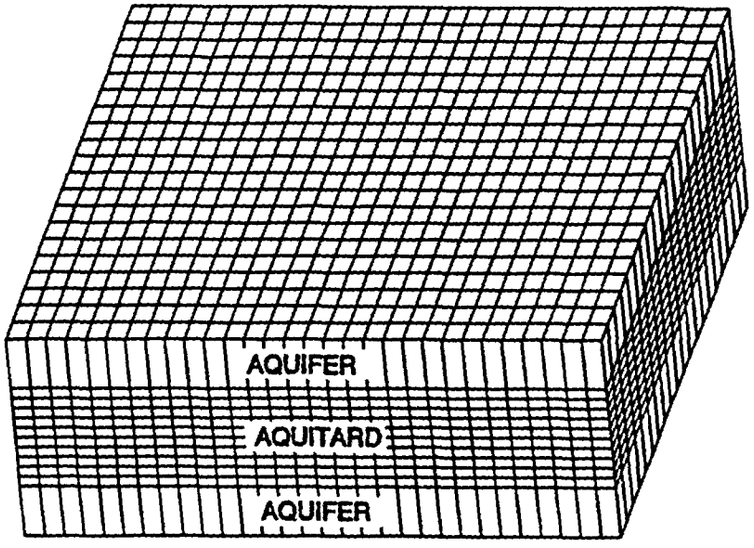


Figure 1. Standard Three-Dimensional Finite-Difference Grid

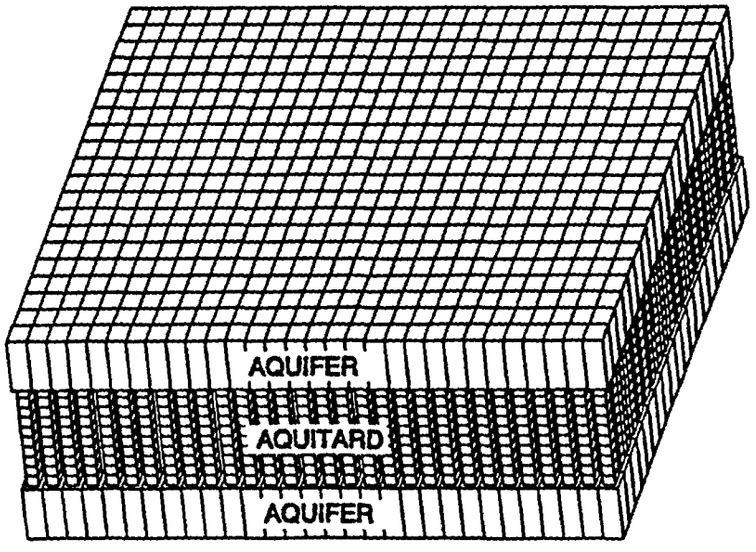


Figure 2. Dynamic Coupling Finite Difference Grid

APPLICATION

To demonstrate the practical benefits of the dynamic coupling technique, a recent modeling study that became feasible only due to dynamic coupling is presented below. This modeling study was conducted to evaluate and to optimize the aquifer remediation plan for a chemical-plant site in Tacoma, Washington. The plant is owned and operated by ATOCHEM North America. Past production and handling of an arsenic-based herbicide termed **Penite** have resulted in arsenic contamination of the groundwater beneath the plant (Figures 3 and 4).

The ATOCHEM North America chemical plant is situated on the peninsula between the Blair and the Hylebos waterways in Tacoma, Washington. Both waterways run into Commencement Bay and Puget Sound. The arsenic contamination is primarily in the unsaturated and saturated zone of the sandy artificial (i.e., dredged) upper aquifer. However, some arsenic has migrated about 0.5 m into the underlying clayey-silt first aquitard. Locally, the arsenic has migrated through the first aquitard into the intermediate aquifer beneath the first aquitard. Contaminated groundwater discharges from the upper and the intermediate aquifers into the Hylebos waterway (Figure 3).

ATOCHEM has developed a **Final Remediation Action Plan (FRAP)** which will provide a longterm solution to the ground-water contamination. The FRAP, which will be implemented and fully operational by late 1992, has two specific objectives: (i) to reduce the arsenic discharge to the Hylebos waterway to 10 % or less of the current loading, and (ii) to remediate the subsurface, i.e., to remove the mobile arsenic from the upper and the intermediate aquifers to the extent technically feasible.

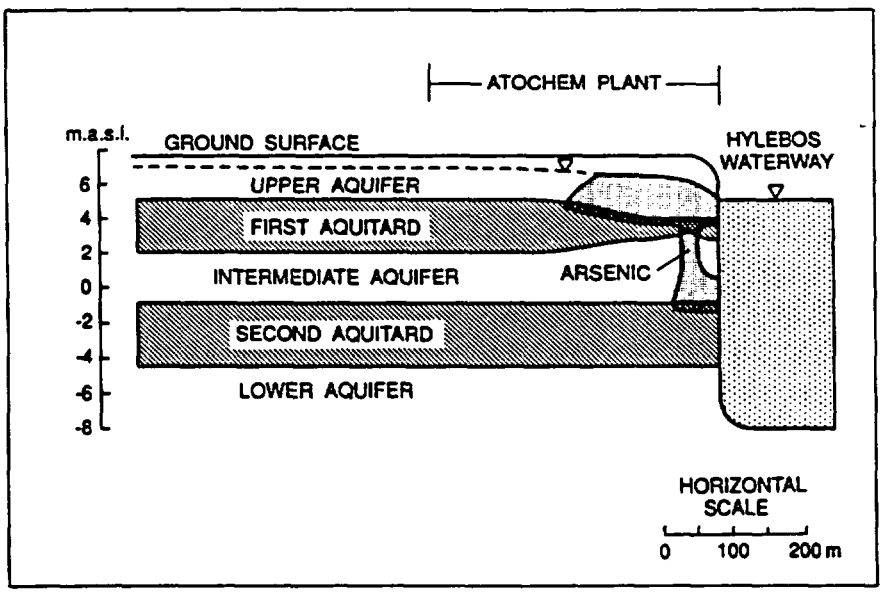
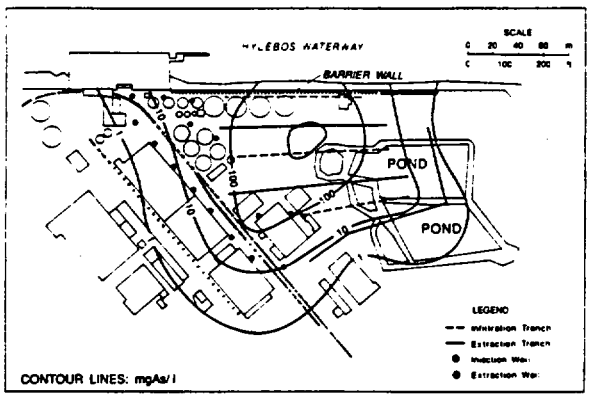


Figure 3. Schematic Extent of the Arsenic Contamination

(a)



(b)

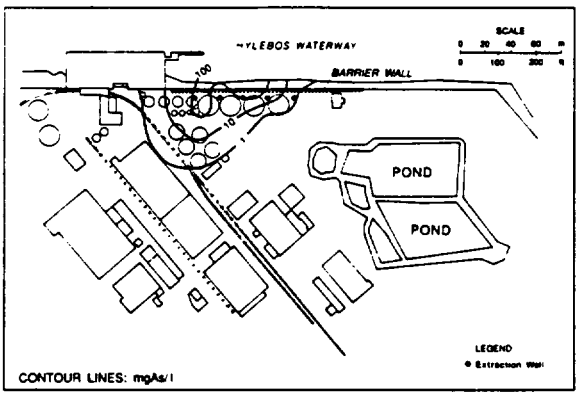


Figure 4. Arsenic Contamination and FRAP Configuration in the Upper Aquifer (a) and in the Intermediate Aquifer (b)

Conceptually, the FRAP comprises two phases: active and passive. During the **active phase**, approximately 10 years, contaminated groundwater will be extracted, treated, and possibly reinjected. In the upper aquifer, the proposed configuration of the hydraulically active elements comprises 6 infiltration/extraction trenches and 14 injection/extraction wells (Figure 4a). In addition, 5 extractions wells will be installed in the intermediate aquifer (Figure 4b). The hydraulically active elements are complemented by a passive barrier wall (continuous sheet piling) through both aquifers along the Hylebos waterway. The primary purpose of the barrier is to mitigate the arsenic discharge to the Hylebos waterway prior to and during the aquifer remediation.

The **passive phase**, with an unspecified time frame, comprises longterm arsenic migration controlled by the natural subsurface hydraulic regime and by the sheet pile structure such that the arsenic discharge limits are not exceeded.

Modeling Approach

The project-specific requirements of the modeling study were to simulate three-dimensional, saturated and unsaturated, ground-water flow and retarded arsenic transport during pre-remediation conditions, during the active phase, and during the passive phase. To meet these requirements with satisfactory horizontal resolution, a combination of three finite-difference models with nested model areas was used (Figure 5). The **regional-scale model** encompasses most of the peninsula between the Hylebos and the Blair waterways. Its primary purpose is to provide the boundary conditions for the **local-scale model**. The local-scale model encompasses an area about twice the size of the ATOCHEM plant between the Hylebos waterway and the center line of the peninsula. This model is used to simulate pre-remediation conditions and the passive phase. It also provides boundary conditions for the smallest of the three models, i.e., the **remediation model**. The remediation model encompasses essentially the area of

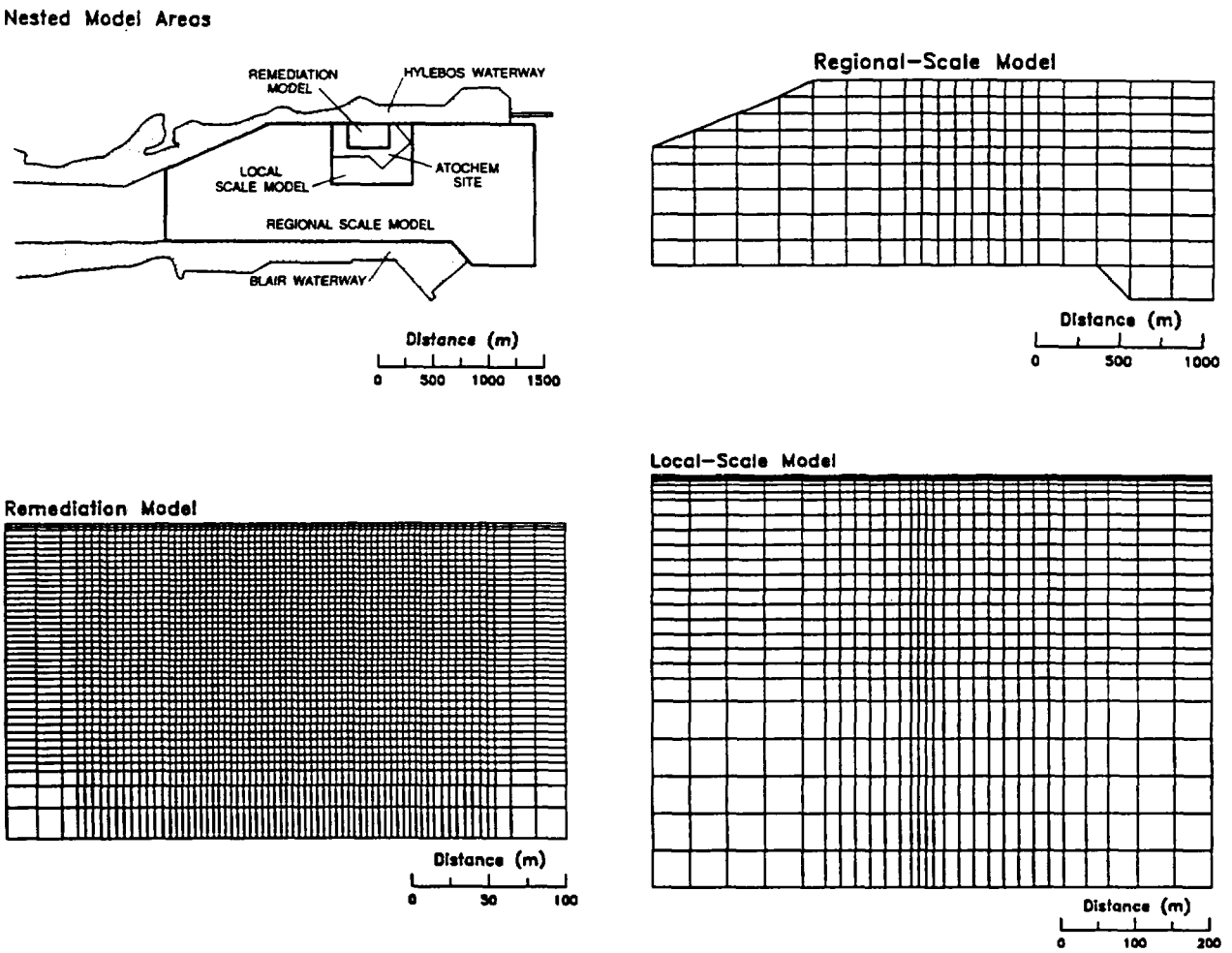


Figure 5. Nested Model Areas and Model Discretizations

present arsenic contamination. It is used to simulate the active-phase remediation process.

Conceptually, a number of processes are essential for accurate characterization of the pre-remediation situation (base case). These include: Primarily horizontal ground-water flow and retarded arsenic transport in the aquifers below the water table; primarily vertical flow and transport in the unsaturated upper aquifer and in the aquitards; recharge into the unsaturated zone of the upper aquifer; and discharge to the Hylebos waterway. In the unsaturated zone, infiltration and retarded arsenic transport to the water table are approximated by using the calibration-derived recharge rate as the vertical flux through the unsaturated zone.

During the active aquifer remediation, injection and extraction are added as processes. Also, beginning with the active phase, the arsenic discharge to the Hylebos waterway is reduced due to the barrier wall. Simulation of the passive phase implements essentially the same processes as the base case simulations.

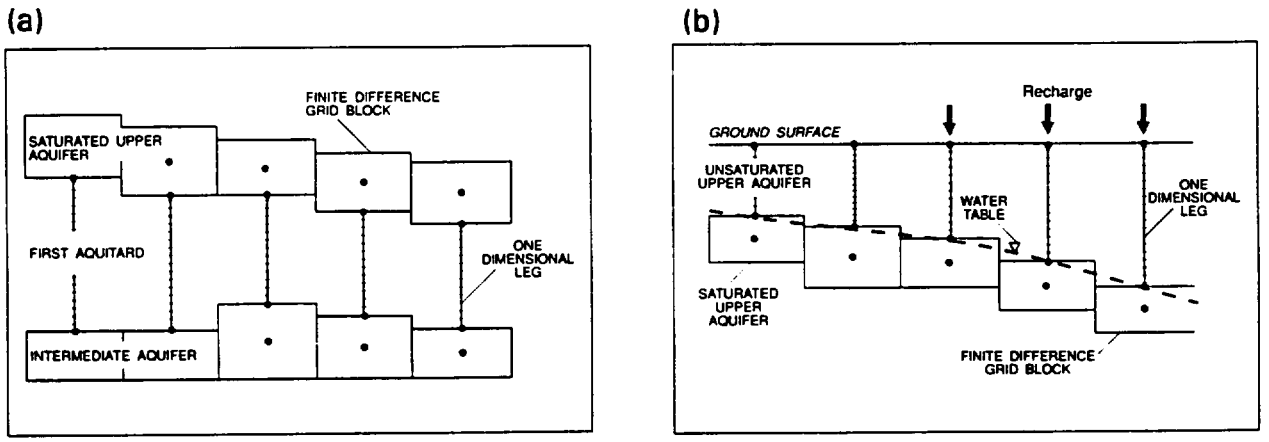


Figure 6. Schematic Discretization of the Aquitards (a) and the Unsaturated Upper Aquifer (b)

As indicated by Figure 5, the resolution of the regional-scale model is between 100 and 200 m. The resolution of the local-scale model and of the remediation model is 10-20 m and 4-5 m, respectively. This increased horizontal resolution allows for adequate simulation of the different processes at the different scales.

The dynamic coupling option of SWIFT II was applied to achieve a satisfactory vertical resolution of the simulated processes. Specifically, the aquitards and the unsaturated upper aquifer were discretized into columns of vertical one-dimensional subgrids (Figures 6a and 6b). As expected, this implementation resulted in a substantial reduction of both the memory requirements and the execution times. The remediation model with 25600 grid blocks requires only 9 MB RAM. On an 80386-based 25-MHz PC, the computing time per time step averaged to 40 seconds.

Simulation of Pre-Remediation Conditions

The pre-remediation processes were implemented into the regional-scale model. The regional-scale model was calibrated against the longterm average water levels measured in more than 50 monitoring wells. The resulting head distribution was then used to establish the boundary conditions of the local-scale model.

Subsequently, the pre-remediation processes were implemented into the local-scale model. To account for the better resolution, the calibration of the local-scale model was refined using again the historic water level measurements from the observation wells. Starting with the current arsenic distribution as initial conditions (Figure 4), the calibrated local-scale model (base case model) was then used to simulate unremediated arsenic discharge and the remaining arsenic in place for a period of 200 years (Figures 7a and 7b). Accordingly, the unremediated arsenic loading to the Hylebos waterway is estimated to be 2400 kg/y, with about 80 % discharging from the upper aquifer.

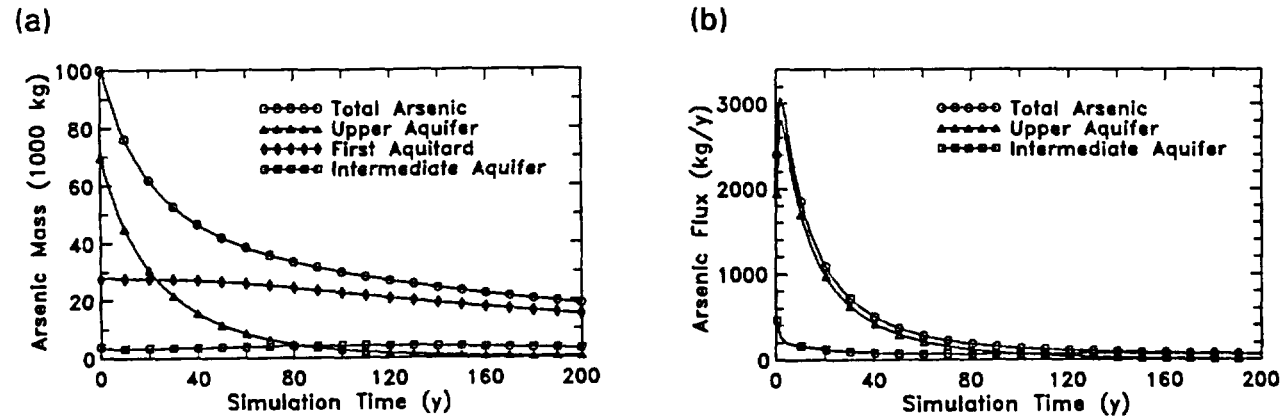


Figure 7. Base Case Simulation: Arsenic in Place versus Simulation Time (a) and Arsenic Discharge to the Hylebos Waterway (b)

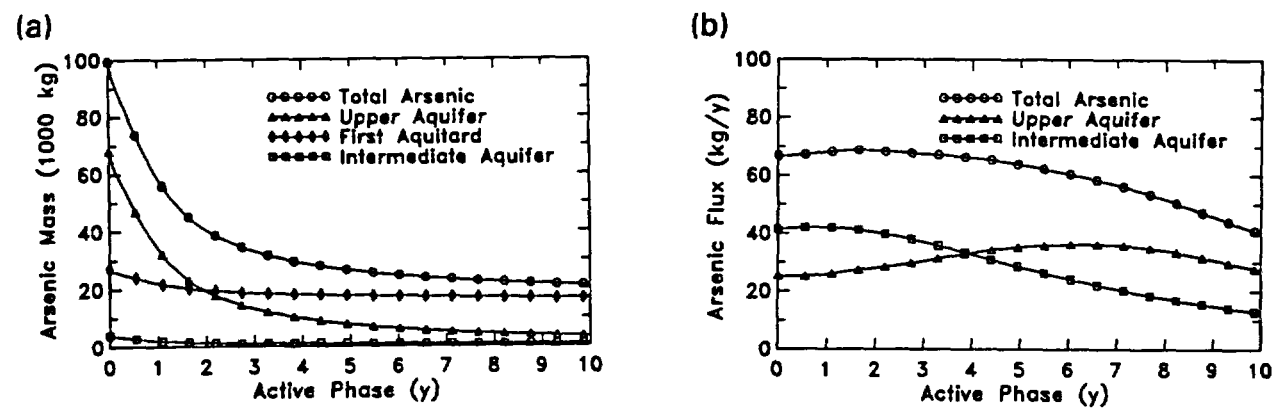


Figure 8. Active Phase: Arsenic in Place versus Simulation Time (a) and Arsenic Discharge to the Hylebos Waterway (b)

Simulation of Active Aquifer Remediation

The active-phase was simulated using the small-scale remediation model. The boundary conditions were established using the flow field of the local-scale model after implementing the barrier wall. Beginning with an initial FRAP configuration, active aquifer remediation was simulated over a period of 10 years. The FRAP configuration (i.e., geometry and extraction/infiltration rates) was step-wise improved until the remediation objectives were met. The resulting FRAP configuration (Figure 4) is predicted to allow removal of about 80 % of the arsenic from the system (Figure 8a). Most of the remaining arsenic will remain relatively immobilized in the first aquitard due to the relatively low aquitard permeability. During the active phase, arsenic discharge to the Hylebos waterway will be reduced to less than 3 % of the unremediated case (Figure 8b). The areal distribution of the arsenic concentrations in the

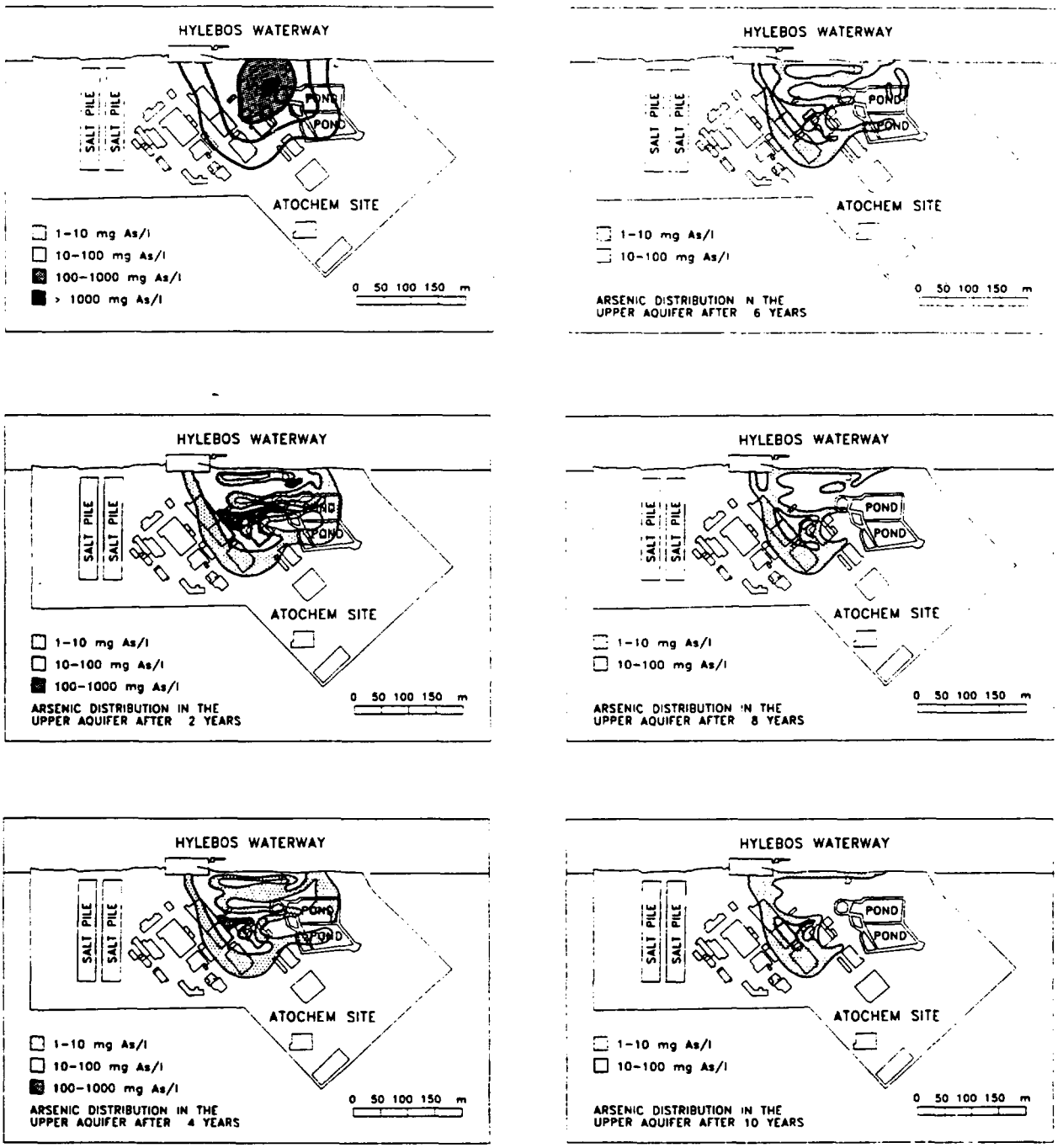


Figure 9. Active Phase: Simulated Arsenic Distributions in the Saturated Upper Aquifer

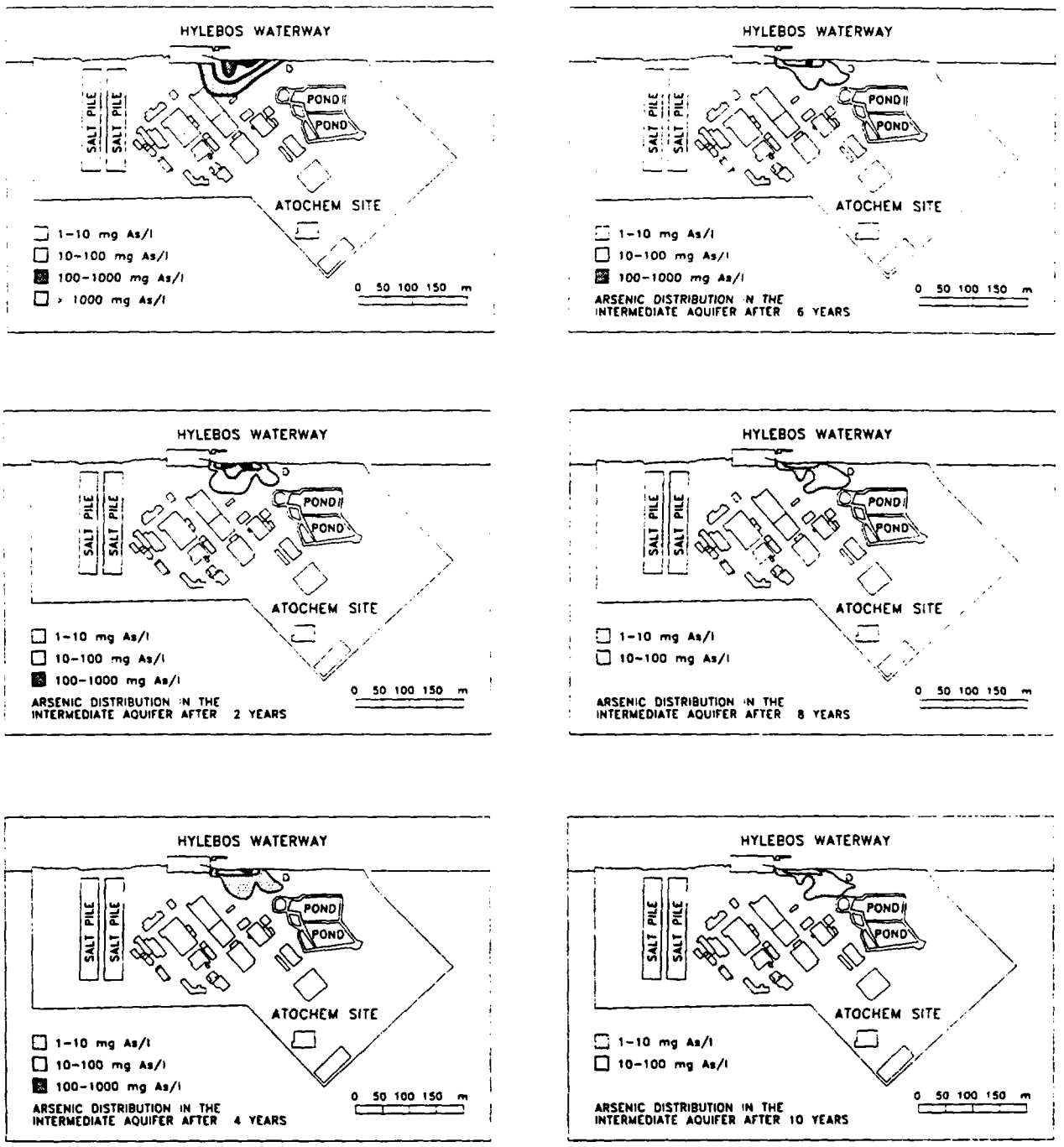


Figure 10. Active Phase: Simulated Arsenic Distributions in the Intermediate Aquifer

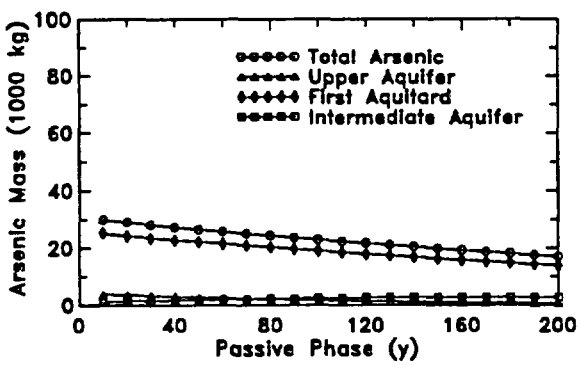
saturated upper aquifer and the intermediate aquifer during the active phase is shown for different simulation times in Figures 9 and 10. The figures indicate that the FRAP configuration is effective in most parts of the contaminated area. The figures further illustrate the increased horizontal resolution obtained by using nested models with increasingly refined grids.

Simulation of Passive Aquifer Remediation

After completion of the active phase, the hydraulic system is expected to return to natural conditions, except for the fact that the sheet-pile structure remains in place. Therefore, the passive phase was simulated using the calibrated base-case model with the barrier wall implemented and the arsenic distribution at the end of the active phase as initial conditions (Figures 9 and 10). The simulations were carried out over a period of 190 years (Figure 11). The predicted arsenic discharge to the Hylebos waterway never exceeds 5 % of the unremediated flux. The proposed FRAP, therefore, achieves the objective of reducing the longterm arsenic flux to the Hylebos waterway to less than 10 % of the pre-remediation flux.

To demonstrate the vertical resolution of the passive-phase simulation, the arsenic concentrations in the first aquitard are shown for different times in Figure 12. The graphs clearly illustrate the slow migration of the remaining arsenic through the first aquitard and into the intermediate aquifer during the first 100 years after completion of the active-phase aquifer remediation.

(a)



(b)

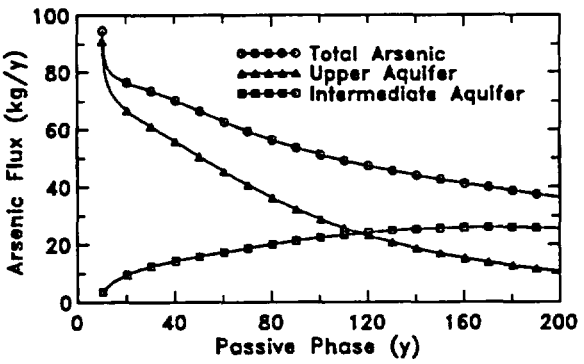
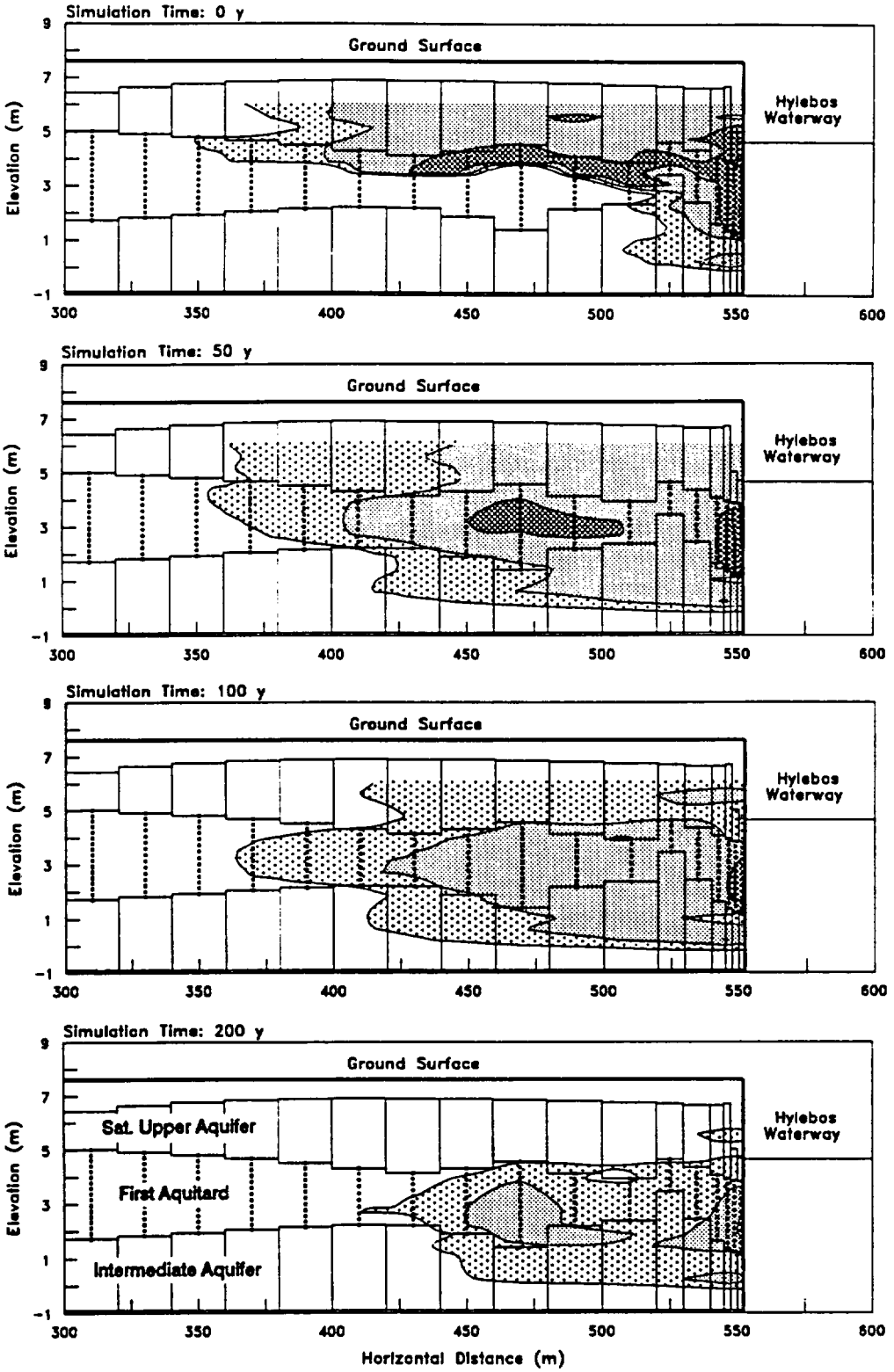


Figure 11. Passive Phase: Arsenic in Place versus Simulation Time (a) and Arsenic Discharge to the Hylebos Waterway (b)



Legend: see Figure 9

Figure 12. Passive Phase: Simulated Arsenic Distributions in the First Aquitard

CONCLUSIONS

Dynamic coupling is a very useful tool for simulating complex hydrogeological situations, especially multi-layered aquifer-aquitard combinations. In such situations, dynamic coupling allows for a sufficiently fine vertical discretization of the aquitards with a given horizontal discretization. With dynamic coupling, model applications become feasible which are almost impossible using standard finite-difference modeling techniques.

Dynamic coupling was successfully applied in a modeling study conducted to evaluate and to optimize the aquifer remediation plan for a chemical plant site. The simulation results indicate that most of the arsenic can be removed from the aquifers during a 10-year pump-and-treat phase. However, a significant amount of arsenic (about 20 %) will remain primarily in the first aquitard. During the first 100 years after completion of the active-phase aquifer remediation, most of this arsenic will slowly migrate through the first aquitard into the underlying intermediate aquifer and eventually discharge into the Hylebos waterway. However, the long-term passive-phase discharge rate is less than 5 % of the unremediated flux.

REFERENCES

Reeves, M., D.S. Ward, N.D. Johns, and R.M. Cranwell, 1986a. Theory and Implementation for SWIFT II, The Sandia Waste-Isolation Flow and Transport Model for Fractured Media, Release 4.84, Sandia National Laboratories, Albuquerque (NM), NUREG/CR-3328 and SAND83-1159.

Reeves, M., D.S. Ward, N.D. Johns, and R.M. Cranwell, 1986b. Data Input Guide for SWIFT II, The Sandia Waste-Isolation Flow and Transport Model for Fractured Media, Release 4.84, Sandia National Laboratories, Albuquerque (NM), NUREG/CR-3162 and SAND83-0242.

Price, H.S., and Coats, K.H., 1973. Direct Methods in Reservoir Simulation, Society of Petroleum Engineers Journal Paper No. 4278, 14 (3), pp. 295-308.