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DETAILED VALIDATION OF A LIQUID AND HEAT FLOW CODE AGAINST FIELD PERFORMANCE

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Authors

Tsang, C.-F.

Doughty, C.

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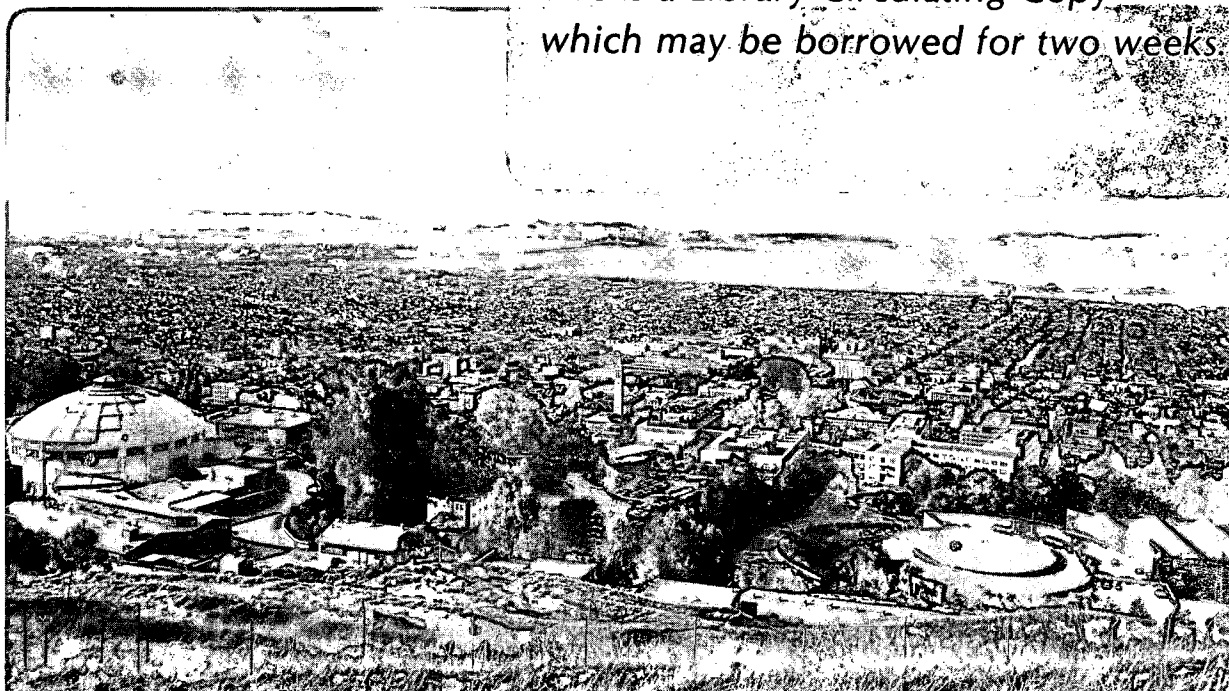
DETAILED VALIDATION OF A LIQUID AND HEAT FLOW
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C.-F. Tsang and C. Doughty

February 1985

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DETAILED VALIDATION OF A LIQUID AND HEAT FLOW
CODE AGAINST FIELD PERFORMANCE

Chin-Fu Tsang and Christine Doughty

Earth Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

February 1985

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ABSTRACT

The numerical code PT, which calculates liquid and heat flow in a saturated porous or fractured porous medium, has been validated against a series of field experiments involving the injection and subsequent production of hot water into a confined aquifer. The layered structure of the aquifer and strong buoyancy effects, indicating highly coupled liquid and heat flows, provide a stringent test of the code's ability to model the real world.

INTRODUCTION

In general, there are two requirements before a numerical code can be accepted as a useful tool. Firstly, it must be verified against analytical solutions in order to show that the governing equations of the mathematical model have been correctly programmed into the code, and the numerical solution algorithm works with adequate accuracy. Secondly, it must be validated against field data in order to check that the mathematical model used properly represents the physical processes taking place.

A three-dimensional numerical code called PT has been developed at Lawrence Berkeley Laboratory¹ to calculate liquid and heat flow through a water-saturated porous or fractured porous medium, based on the Integrated-Finite-Difference method^{2,3}. The code PT can handle heterogeneous and anisotropic materials, complex boundary conditions, temperature dependent properties, variable strength sources and sinks, and gravitational effects (buoyancy). Flow through fractures is studied by detailed discretization of each fracture; it can be included easily if only a few fractures need to be considered. So far PT has been verified against over eight analytical and semianalytical solutions, including a thermal front tilting problem and two fractured porous medium problems.

Between 1979 and 1983, a comprehensive field validation study of the code PT was carried out. The field experiments were performed by Auburn University^{4,5,6,7}; they involved multiple cycles

References and illustrations at end of paper.

of injection, storage, and production of hot water in a shallow confined aquifer. The temperature field in the aquifer was monitored by a number of observation wells completed with thermistors at multiple depths. Five injection-storage-production cycles were carried out by Auburn University in close coordination with modeling calculations done with the code PT by Lawrence Berkeley Laboratory. The validation of the code was carried out in several stages: (1) history matching of the first two injection-storage-production cycles; (2) a double-blind prediction of the third and fourth cycles (calculated results were compared with field data only after each cycle had been completed); (3) optimization studies of alternative injection-production designs for the fifth cycle and subsequent comparison with experimental data of the fifth-cycle. In the course of the validation studies we also carried out parameter sensitivity studies to identify critical parameter groups and discovered that a region of the aquifer has a layered structure. The interplay of forced convection, natural convection, the layered structure of the aquifer, and the temperature dependence of fluid properties provides a very stringent test of our computer code.

This paper reviews these validation studies and points out key features of a properly designed validation procedure for a complex heat and fluid flow computer code.

THE COMPUTER CODE PT

The computer code PT is capable of calculating coupled liquid and heat flows in a water-saturated porous or fractured porous medium. The governing equations for PT consist of the conservation equations for mass and energy, and Darcy's law for fluid flow. Pressure and temperature are the dependent variables. One-dimensional consolidation of the rock matrix can be considered as well, using the theory of Terzaghi⁸. The mass and energy conservation equations are coupled through the fluid flow in the convection term of the energy equation, and the pressure and temperature dependent fluid and rock properties. The rock matrix and fluid are considered to be in local thermal equilibrium at all times. Energy changes due to fluid compressibility, acceleration, and viscous dissipation are neglected.

The following physical effects are included in PT calculations: (1) heat convection and conduction; (2) regional groundwater flow; (3) multiple heat and/or mass sources and sinks; (4) constant pressure or temperature boundaries; (5) hydrologic or thermal barriers; (6) gravitational effects (buoyancy); (7) complex geometries due to heterogeneous materials; and (8) anisotropic permeability and thermal conductivity.

PT carries out the spatial discretization of the flow regime using the Integrated-Finite-Difference method. This method treats one-, two-, or three-dimensional problems equivalently. An efficient sparse solver⁹ is used to solve the linearized mass and energy matrix equations. The equations are solved implicitly to allow for large time steps. PT adjusts the time step automatically, so that the temperature or pressure change in any node during one time step is within user-specified limits. Mass and energy balances are calculated for each node every time step.

PT has been verified against the following analytical solutions: (1) Theis problem¹⁰; (2) Cold water injection into a hot reservoir¹¹; (3) The temperature variation at a production well due to cold water injection¹²; (4) Radial conduction outside a constant temperature cylinder¹³; (5) Two-node problem, transient conduction heat transfer between two adjacent blocks; (6) The rate of thermal front tilting when hot water is injected into a cold reservoir¹⁴; (7) Pressure response in a well intercepting a finite conductivity vertical fracture¹⁵; (8) Pressure response in a well intercepting a (uniform flux) horizontal fracture¹⁶. As can be seen, each analytical solution isolates one or two of the effects calculated by PT. Field validation, on the other hand, incorporates a number of highly coupled processes.

APPROACH TO FIELD VALIDATION

The field validation of the numerical code PT proceeded in several stages. First, PT was used to do a history match of the first two cycles of the field experiment. All data from the experiment were available to the modelers. Second, PT was used to make a double-blind prediction of the next two cycles of the field experiment. Only the design parameters of the experiment were available to the modelers, not any results. Third, PT was used to do optimization design studies for a planned cycle of the field experiment, and subsequently results of the actual cycle were compared with the PT calculations. Progressing from each stage to the next provided a more stringent test of the numerical model, as the code was used more and more as a predictive tool. At each stage of the validation, a number of parameter sensitivity studies were done, in order to determine which parameters affected the results of the experiment most significantly. Study of the discrepancies between the calculated and observed field results gave insight into possible physical processes not included in the numerical model, and provided direction for future work on model development.

HISTORY MATCH

The Water Resources Research Institute of Auburn University conducted a two-cycle injection-

storage-production field experiment on a shallow aquifer in northeastern Mobile County, Alabama in 1978. A single injection/production well was screened in the upper half of a confined 21-m-thick aquifer. The aquifer matrix consists primarily of medium to fine sand, with approximately 15 percent interstitial silt and clay. The aquifer is located from about 40 to 61 m below the land surface and is capped by a 9-m-thick clay sequence; it is bounded below by another clay sequence of undetermined thickness. Above the upper clay unit lies another aquifer, which provided the injection water. A number of observation wells were located around the injection/production well; each was completed with thermistors that measured temperature at six depths in the aquifer. Each injection-storage-production cycle lasted six months and involved the injection and recovery of about 55,000 m³ of water heated to an average temperature of 55°C. The ambient water temperature of the supply and storage aquifers was 20°C. A convenient quantitative measure of each cycle is the recovery factor, defined as the ratio of the energy produced to the energy injected when equal volumes have been produced and injected, with energies measured relative to the ambient groundwater temperature. The first-cycle recovery factor was 0.66 and the second-cycle recovery factor was 0.76.

Well tests were done to determine the hydraulic properties of the aquifer, and laboratory tests made on samples to determine thermal properties of the aquifer and clay layers. Several of the material properties needed for the numerical calculation were not provided, in these instances reasonable values from the literature were used. Whenever possible, sensitivity studies were done to examine the effect of the variation of such parameters. Table 1 summarizes the material properties used for the different layers. Field measurements indicated very small regional groundwater flow, so an axisymmetric model was devised for the calculation. The spatial discretization for a model considering combined heat and fluid flow from a central well must be done with care. For the pressure calculation, the size of the nodes should logarithmically increase with increasing radial distance from the injection well; for the temperature calculation, the size of the nodes should decrease. A compromise of equally spaced nodes within the region of thermal influence, about 60 m, was used. Beyond this region, the size of the nodes steadily increased out to a distance of 20 km where there was a constant pressure boundary. The vertical spacing of the nodes was made fine wherever sharp gradients in temperature were expected, such as at the bottom of the well screen, and in the clay layers adjacent to the aquifer. To assure that the spatial discretization (the calculational mesh) was adequate for the problem, alternate meshes were devised and used for parts of the first cycle calculation, and results compared to results from the primary mesh. Figure 1 shows a vertical section of the central portion of the primary mesh.

After the calculation for each cycle was carried out, the calculated temperature distributions in the aquifer at various times were compared to measured temperatures¹⁷. The overall match was very good, however the calculated temperature profiles, shown in Figure 2, appeared to be sharper than the observed ones, indicating that the mathe-

mathematical model underpredicted thermal diffusion. This is because the model did not include the heterogeneities of the real aquifer that caused fingering, leading to a diffuse front. By comparing the calculated temperatures with temperatures from observation wells located in different directions from the injection/production well, some deviation from axisymmetry was noted. However, the calculated temperature of the produced water agreed very closely with the observed data, as shown in Figures 3 and 4. The production temperature provided an integrated result of the cycle, as the production temperature is the average temperature of water from all directions around the injection/production well. The time-average of the production temperature is proportional to the recovery factor. PI calculated recovery factors of 0.68 and 0.78 for the first and second cycles, respectively, as compared to experimental values of 0.66 and 0.76. This excellent agreement indicated that the small heterogeneities of the system tended to balance out, and that on the whole an axisymmetric model of the system was appropriate.

One of the properties of the aquifer not determined by the well tests was the permeability anisotropy, the ratio of vertical to horizontal permeability in the aquifer. A value of 0.10 was chosen for the model, based on previous modeling studies done at this site¹⁸. A sensitivity study was carried out for the first cycle using values of 1.0 and 0.02 for permeability anisotropy. For the smaller value of anisotropy (i.e. smaller vertical permeability) there was less buoyancy flow of the injected water than in the original first cycle calculation, resulting in a more compact hot plume with lower surface to volume ratio. This led to smaller conductive heat losses, hence a higher recovery factor--0.71. For the larger value of anisotropy, buoyancy flow was increased, creating a more elongated plume with larger heat losses, leading to a recovery factor of 0.57. The large variation in recovery factor indicated that the permeability anisotropy is an important parameter when field data is being modeled.

In the mesh variation studies described above a fine mesh with half the radial spacing of the primary mesh and a coarse mesh with double the radial spacing were used to calculate the temperature distribution in the aquifer at the end of the first-cycle injection period. As shown in Figure 5, the temperature profiles of the fine and primary meshes were quite similar, while those of the coarse mesh were somewhat less sharp, indicating that a small amount of numerical diffusion was present to broaden the temperature front. The calculation using the coarse mesh resulted in a recovery factor of 0.67, just slightly less than that calculated with the primary mesh, and closer to the experimental value. One possible explanation is that the numerical dispersion acted like physical dispersion, caused by aquifer heterogeneities, to broaden the thermal front, increasing heat losses, and lowering recovery factor.

In summary, the history match indicated that the numerical code PI and an axisymmetric model could match the results of the injection-storage-production cycles very well. Detailed comparisons with individual wells showed some discrepancies, but they tended to cancel out when integrated results

such as production temperature and recovery factor were considered. A parameter study indicated that the permeability anisotropy is a very important parameter affecting the results of the experiment. The mesh variation demonstrated the range of mesh spacing appropriate for this particular problem, and showed that numerical dispersion may mimic physical dispersion caused by aquifer heterogeneities.

DOUBLE-BLIND PREDICTION

In contrast to the history match, in which all the experimental results were available to us throughout the course of the modeling study, in the double-blind prediction, we were provided with only the basic geological, well test, injection flow rate and injection temperature data, and the planned production flow rate. We did numerical simulations to predict the outcome of each cycle before its conclusion. During the course of the study, we were not informed of the experimental observations and the experimenters were not informed of our calculated results. Thus we call this a "double-blind" prediction. It was only after both parties concluded their work that detailed comparisons between the calculated and experimental recovery factors, production temperatures, and in situ temperature distributions were made. Our double-blind prediction studies were carried out in the following fashion.

The third, fourth, and fifth cycles of the Auburn experiments were conducted between 1981 and 1982 in a new area of the aquifer, located about 120 m from the site of the first and second cycles. A fully penetrating injection well was used. Rather than using water from the overlying aquifer, a supply well penetrated the storage aquifer itself, creating an injection-supply doublet. During the third cycle, 25,000 m³ of water at an average temperature of 59°C was injected over a period of one month. It was then stored for one month and subsequently produced. During the fourth cycle, a total of 58,000 m³ of water at an average temperature of 82°C was injected over a period of 4.5 months, then stored for one month. Production began using a well screen open to the full aquifer thickness, after two weeks production stopped and the well screen was modified to withdraw water from only the upper half of the aquifer. Production was then resumed and continued until the total water volume produced equaled the volume injected.

Parameter studies done during the first and second cycle history match indicated that the temperature field was not very sensitive to the pressure field in the aquifer, so that in the development of a numerical grid for the later cycles emphasis was placed upon calculating the temperature distribution accurately. An estimate of the radial extent of the hot region in the aquifer around the injection well, the thermal radius, can be made based on conservation of energy. The thermal radius was calculated to be about 25 m for the third cycle and 38 m for the fourth cycle. These values are small compared to the doublet spacing (240 m) and large compared to displacement caused by regional flow, so an axisymmetric model of the aquifer system centered at the injection/production well was used for the calculation. The well bore was modeled by a column of nodes 0.1 m wide with a porosity of 1 and

a very high vertical permeability. Injection and production were accounted for by a source or sink element connected to the top well bore node. Well tests conducted prior to the third cycle included a test to determine vertical permeability in the aquifer. A value of 0.15 was determined for the permeability anisotropy, and used in the mathematical model. Other material properties remained similar to those shown in Table 1.

The third-cycle calculation predicted a recovery factor of 0.61. After reporting this result, along with calculated temperature distributions in the aquifer at various times and the production temperature curve, the experimental results were reported to us. The experimental recovery factor of 0.56, although somewhat below the calculated value, indicated an acceptable prediction. However, the experimental temperature distributions in the aquifer at the end of the injection period appeared rather different from the calculated results, as shown in Figure 6, where two experimental plots show perpendicular cross sections through the aquifer. Apparently, there is a high-permeability layer in the middle of the aquifer into which the injected fluid preferentially flows. After some parameter studies, we chose a three-layer-aquifer model in which the middle layer has a permeability 2.5 times that of the upper and lower layers to represent the system. This three-layer-aquifer model reproduced the experimental temperature distributions and production temperature quite well, as shown in Figures 6 and 7, and predicted a recovery factor of 0.58, much closer to the experimental value than the previous one-layer-aquifer model predicted. This is significant because layering is difficult to detect through conventional well test analysis, which typically gives a single average permeability value for a heterogeneous medium.

The fourth-cycle predictive calculation was made with the three-layer-aquifer model also. This cycle involved injection of much hotter water, at 82°C, than had been used before. Calculated results¹⁹ indicated that for this large temperature, buoyancy effects were very large, and overshadowed the preferential flow into the high permeability layer. Based on the original production plan, which called for a fully penetrating production well, the recovery factor was calculated to be 0.40. However, due to low production temperatures, the experimenters modified the production well during the production period, to eliminate production from the lower half of the aquifer. By following this procedure, the calculated recovery factor was 0.42, as compared to the experimental value of 0.45. This agreement was acceptable, but a comparison of the experimental and calculated production temperature curves, shown in Figure 8, indicated a moderate discrepancy. The calculated production temperature started about 10°C higher than the experimental value, but decreased much more rapidly, so that by the time of the well modification, it underpredicted the experimental temperature. When production resumed after the two days of well modification, the calculated result again overpredicted the experimental value, although by just 2°C. Again the calculated temperature decreased more rapidly than the experimental curve, and ended up underpredicting it. This discrepancy of production temperatures was most noticeable for the fourth cycle, but the pattern of early overpredic-

tion followed by late underprediction was evident in the third-cycle production temperature curves as well. It was much smaller for the first and second cycles, suggesting that it might be related to the well bore model, which was first incorporated in the model for the third-cycle calculation.

In summary, the double-blind prediction made by PT yielded reasonable results. The third-cycle comparison of one-layer and three-layer aquifers indicated the importance of aquifer layering. The fourth-cycle well modification provided information on the effect of well open interval. The higher injection temperature of the fourth cycle caused buoyancy flow to be a dominant effect in the aquifer for the first time. PT can adequately model the fourth cycle, although there is a larger discrepancy between the calculation and the experiment than for the earlier cycles.

OPTIMIZATION DESIGN STUDIES

Because of the decrease in recovery factor from the third to fourth cycles (0.56-0.45) corresponding to the increase in injection temperature, an optimization design study was done before the fifth cycle of the field experiment in an attempt to design an experiment that would yield an optimal recovery factor for an 80°C cycle lasting a total of three months. A series of injection-production schemes using different well-screen open intervals were simulated. Each assumed a constant injection flow rate of 112 gpm (7 kg/sec) at 82°C. The three-layer-aquifer model developed for the third-cycle calculation was used. Two variations in cycle design were considered: the first assumed injection, storage, and production periods of one month each; the second assumed a two month injection period (resulting in double the volume of hot water injected), no storage period, and a one month production period (at double the injection flow rate). Making use of the results of the fourth cycle calculation, which indicated that buoyancy flow had a dominant effect on the system, three general approaches were taken in the design studies (Figure 9): (A) simply inject into and produce from the upper portion of the aquifer where most of the hot water would naturally flow because of buoyancy effects; (B) attempt to maintain a compact shape for the injected fluid--buoyancy flow is counteracted by pumping from the bottom of the aquifer as hot water is injected into the top; and (C) inject into the upper portion of the aquifer, then while producing from the upper portion, produce (and discard) colder water from the lower portion of the aquifer through a "rejection well" located next to the injection/production well, thus eliminating any upward flow of cool water that would lower production temperature. Table 2 summarizes the results of the calculations. The reference case considered an injection/production well screened over the entire aquifer thickness. For a cycle consisting of one month each of injection, storage, and production, the maximum recovery factor was about 0.52, representing an improvement of about 0.12 over the reference case. For the larger injected volume a recovery factor of 0.66 was possible. Hence for this system, the volume of fluid injected was as important as the manner in which it is injected and produced. In general, method C appeared to be most successful in yielding a high recovery factor.

After the optimization design studies were completed, the fifth cycle was carried out, using 80°C water and an injection-production scheme patterned after case C. The injection/production well was screened over the upper 9 m of the aquifer and the rejection well, located less than 2 m away, was screened over 9 m in the lower half of the aquifer. Instead of a three month cycle storing 18,000 or 36,000 m³, as in the design studies, the fifth cycle lasted seven months, and injected 56,700 m³ of water, making a direct check of the design study calculations impossible. The recovery factor for the fifth cycle was 0.42. A history match calculation yielded a recovery factor of 0.44. As in the case of the fourth cycle, the calculated production temperature, shown in Figure 10, initially overpredicted the experimental value, then decreased more rapidly, and finally underpredicted it. The calculated temperature from the rejection well consistently underpredicted the experimental value, indicating that the model may have overpredicted buoyancy flow somewhat. This finding was consistent with the larger production-temperature discrepancy noted for higher temperature (greater buoyancy flow) cycles.

In summary, the optimization design studies described a variety of possible injection-production schemes, and indicated the range of recovery factors for them. Although the actual fifth cycle was quite different than the design studies, the relative results of the design studies proved to be useful in the choice of the fifth-cycle injection-production scheme.

GENERAL DISCUSSION AND CONCLUSIONS

To demonstrate that a sophisticated numerical code is a useful and convincing tool requires considerable effort, but it is an important task in view of the increasing frequency with which numerical models are depended upon to yield results that critically influence significant and costly decisions. A proper validation of a numerical code requires not only verification against analytical or semianalytical solutions, but also detailed field validation studies, as described in this paper by a particular example.

The history match is only the first stage of a validation process. The goal is not a perfect match, but a match that meets the accuracy required for decision-making purposes, with discrepancies that are understood. A discrepancy can represent not only an inaccurate solution procedure, but a failure of the basic formulation of the problem to include a certain physical effect. Sometimes a careful study of the discrepancy can point to new phenomena and open up new directions of research. The double-blind prediction studies ensure that there are no hidden fitting parameters, and avoid subconscious (or otherwise) influence of final results on the calculations. Success in this effort gives confidence in the capability of the code to predict the future behavior of the system studied. Optimization studies demonstrate the flexibility of the code to address alternative scenarios and arrangements, and yield results that are of practical importance to experimental design.

In this paper we described the steps that were taken in the field validation of the code PT.

Because of this study we have considerable confidence in its capability and accuracy. Of course, even with the best code, an experienced and capable user is essential.

ACKNOWLEDGEMENT

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Table 1. Parameters used in the history match calculation.

Formation thickness	Aquifer	21 m
	Aquitard	9 m
Thermal conductivity	Aquifer	2.29 J/m s °C
	Aquitard	2.56 J/m s °C
Heat capacity of rock		1.81×10^6 J/m ³ °C
Density of rock		2600 kg/m ³
Aquifer horizontal permeability		0.53×10^{-10} m ² (53 darcies)
Vertical to horizontal permeability ratio		1:10
Aquitard to aquifer permeability ratio		10^{-5}
Porosity	Aquifer	0.25
	Aquitard	0.15
Storativity	Aquifer	6×10^{-4}
	Aquitard	9×10^{-2}

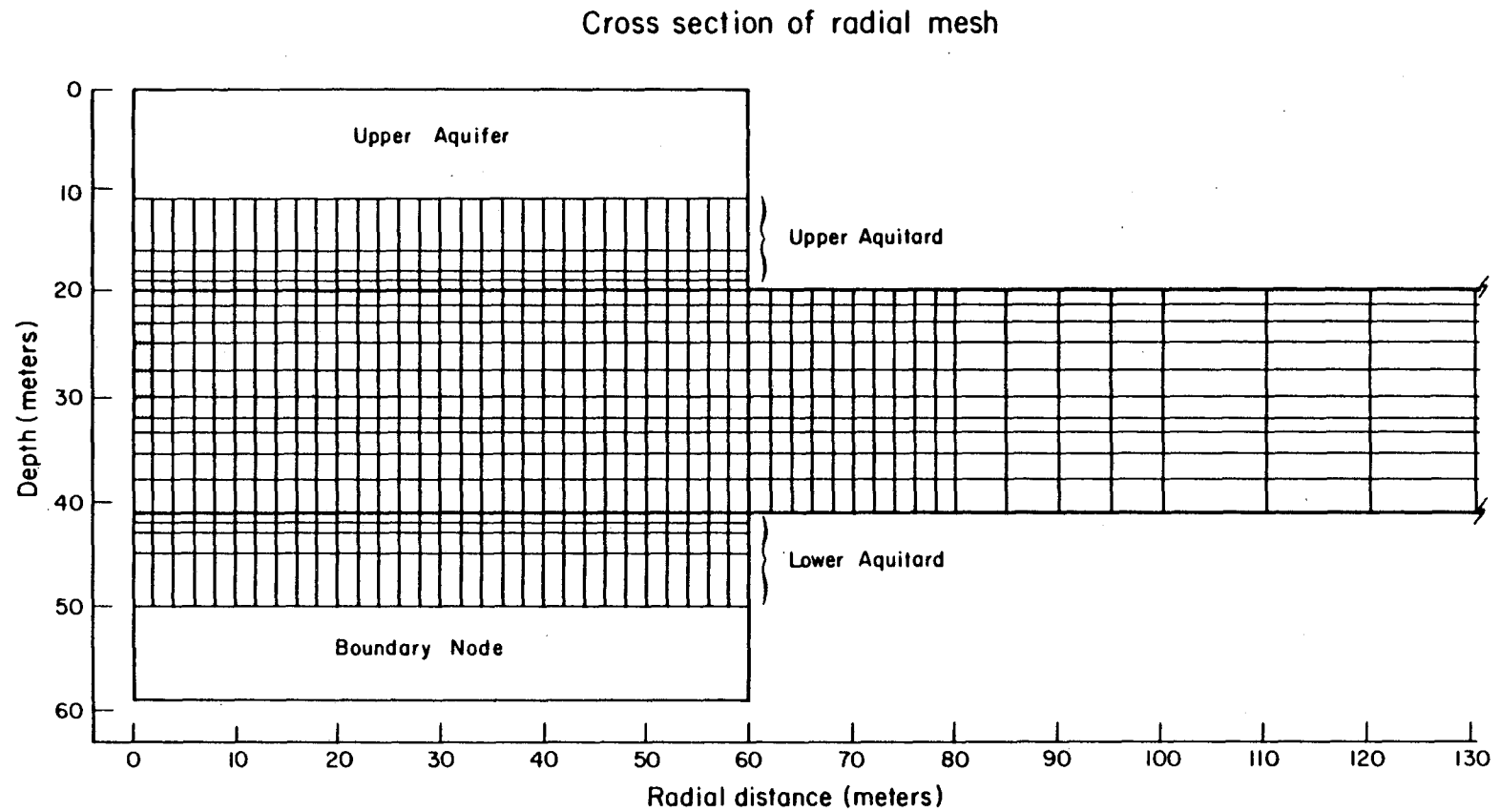
Table 2. Fifth-cycle design studies.
 $T_1 = 82^\circ\text{C}$, $Q = 112$ gpm

I. One month each, injection,
 storage, production
 $V = 18,300 \text{ m}^3$

Case	Well Screen Interval		Recovery Factor
	Injection Period	Production Period	
Ref.	Full	Full	0.404
A1	Upper 40%	Upper 40%	0.448
A2	Upper 40%	Upper 20%	0.501
B1	Upper 20%	Upper 20%	0.516
	Lower 20%		
B2	Upper 20%	Upper 20%	0.487
	Lower 20%	Lower 20%	
C1	Upper 40%	Upper 40%	0.500
		Lower 55%	
C2	Upper 40%	Upper 20%	0.521
		Lower 55%	

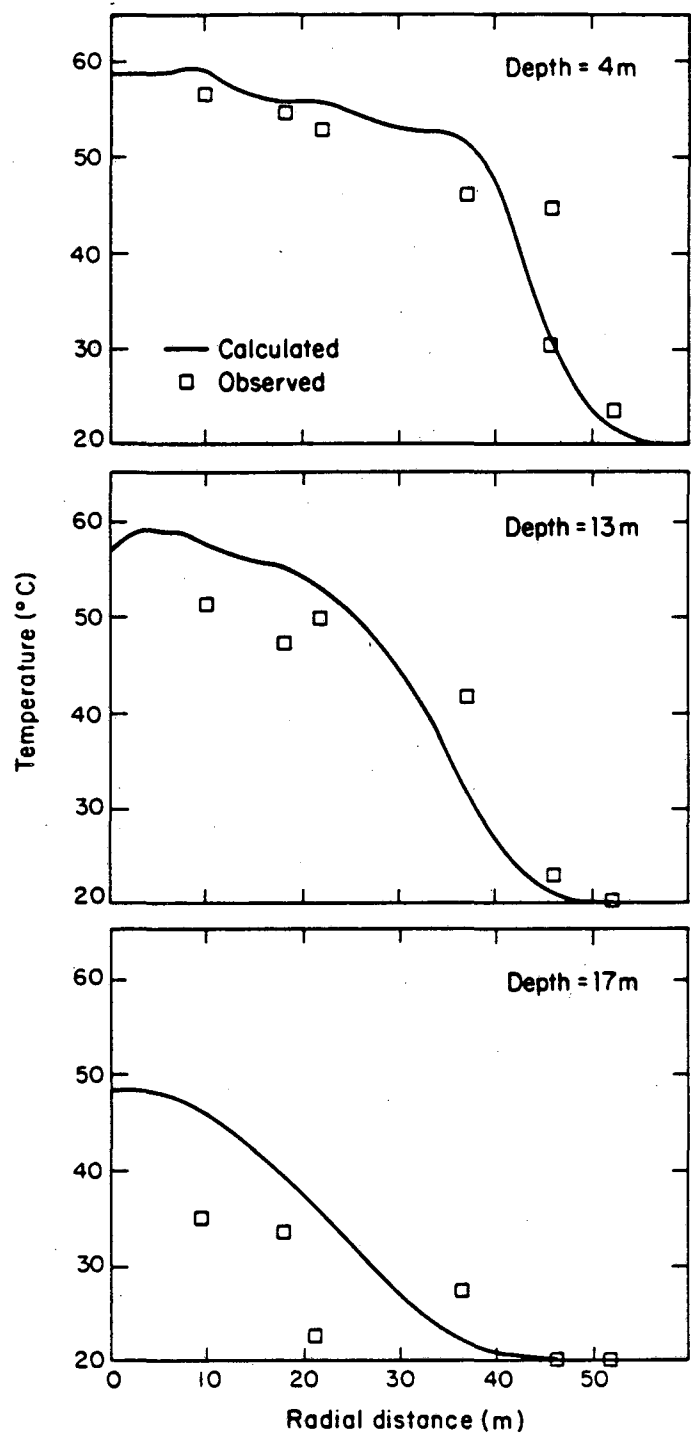
II. Two months injection, one month
 production
 $V = 36,600 \text{ m}^3$, $Q_p = 2Q_i$

A1	Upper 40%	Upper 40%	0.609
C1	Upper 40%	Upper 40%	0.629
		Lower 55%	
C3	Upper 40%	Upper 40%	0.631
		Lower 20%	
C4	Upper 40%	Upper 20%	0.661
		Lower 20%	



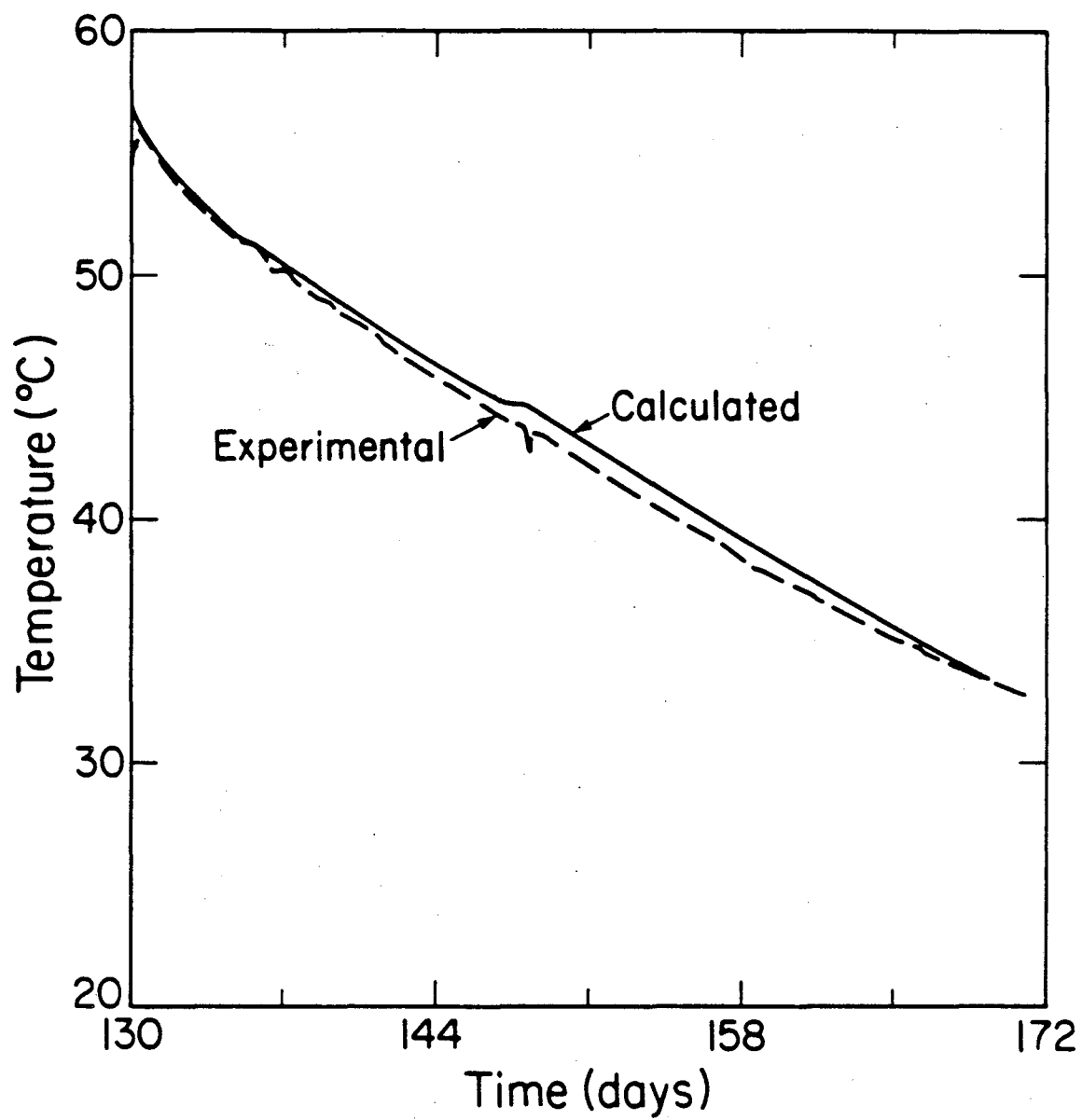
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Fig. 1. Mesh used for the first and second cycle calculation.



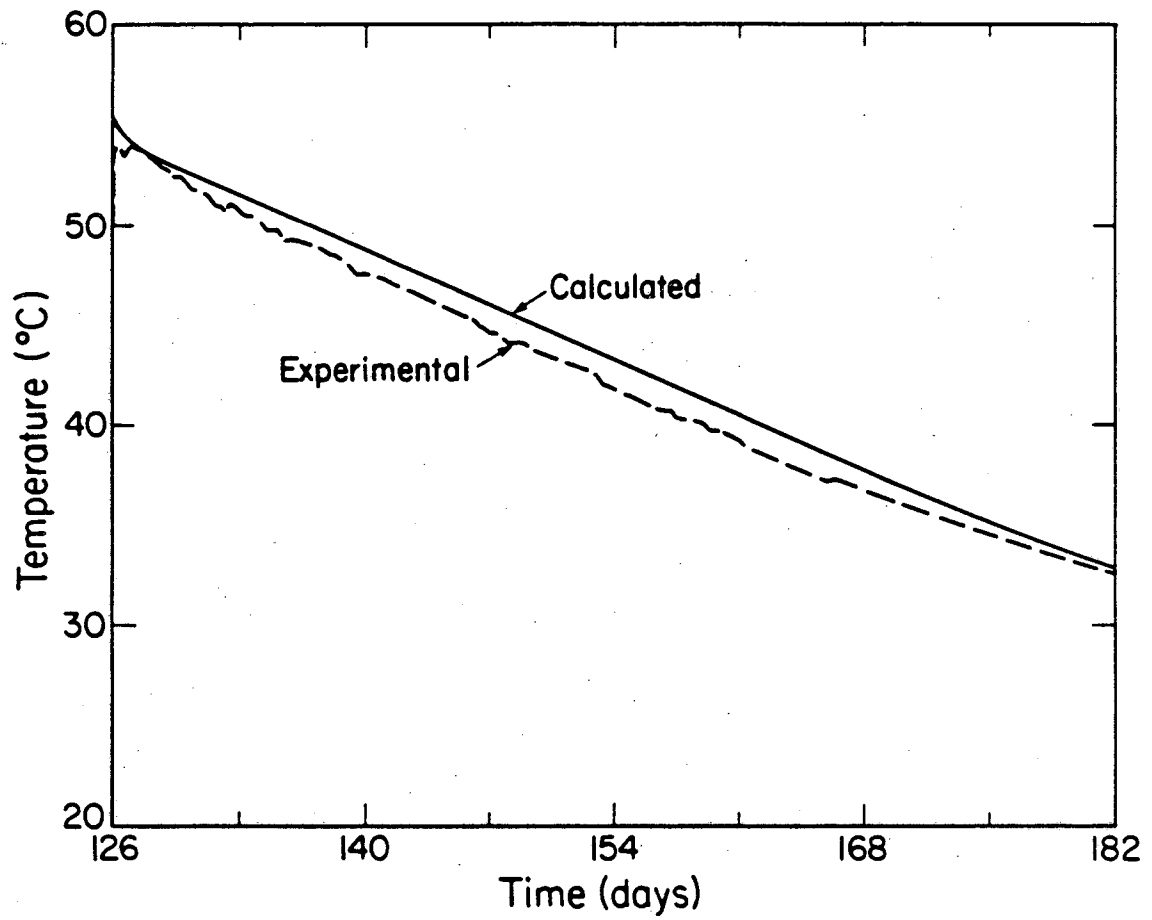
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Fig. 2. Temperature profiles after the first-cycle injection period.



XBL 8412-6195

Fig. 3. First-cycle production temperature.



XBL 8412-6194

Fig. 4. Second-cycle production temperature.

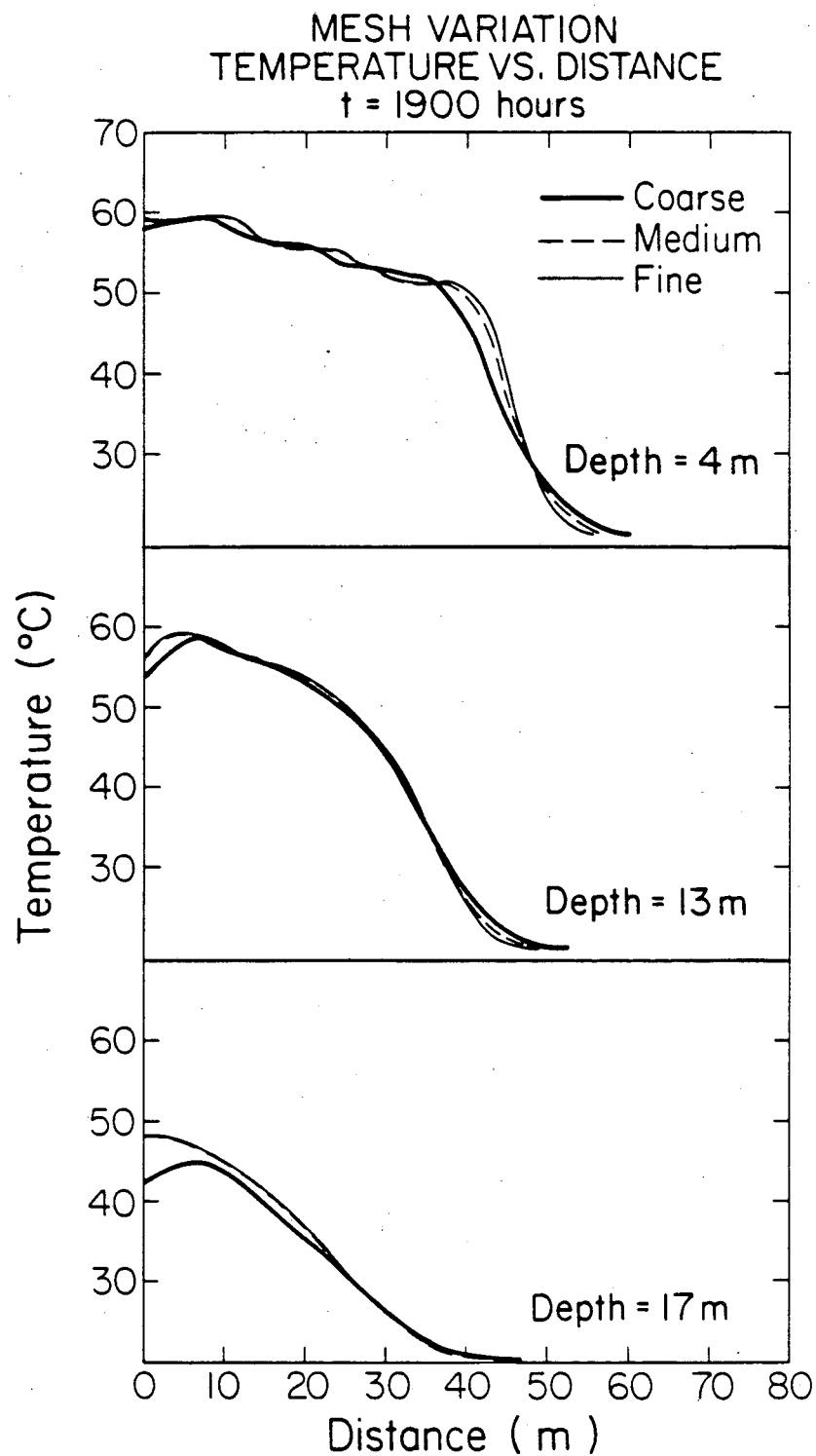
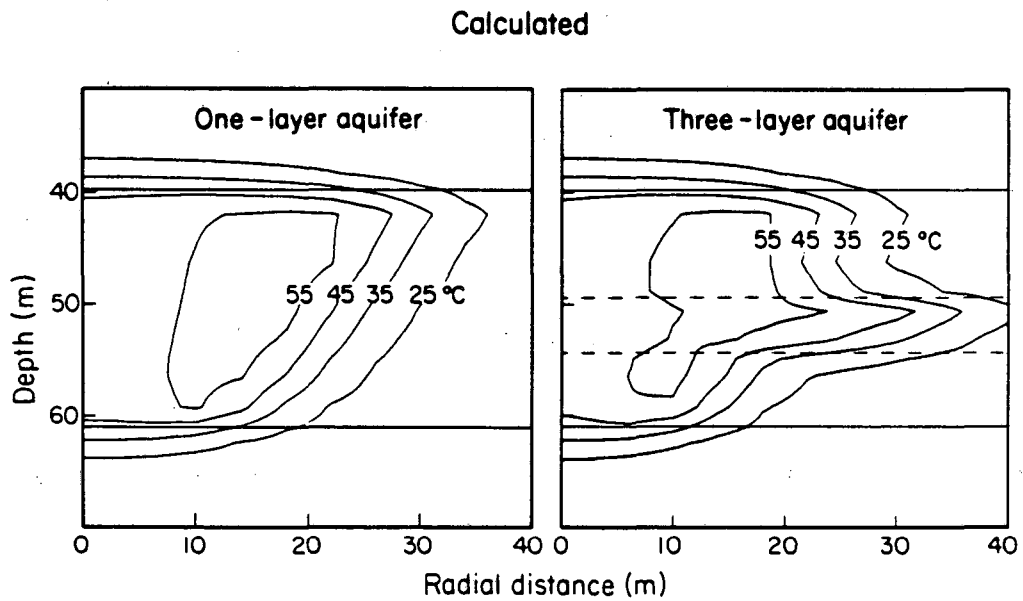
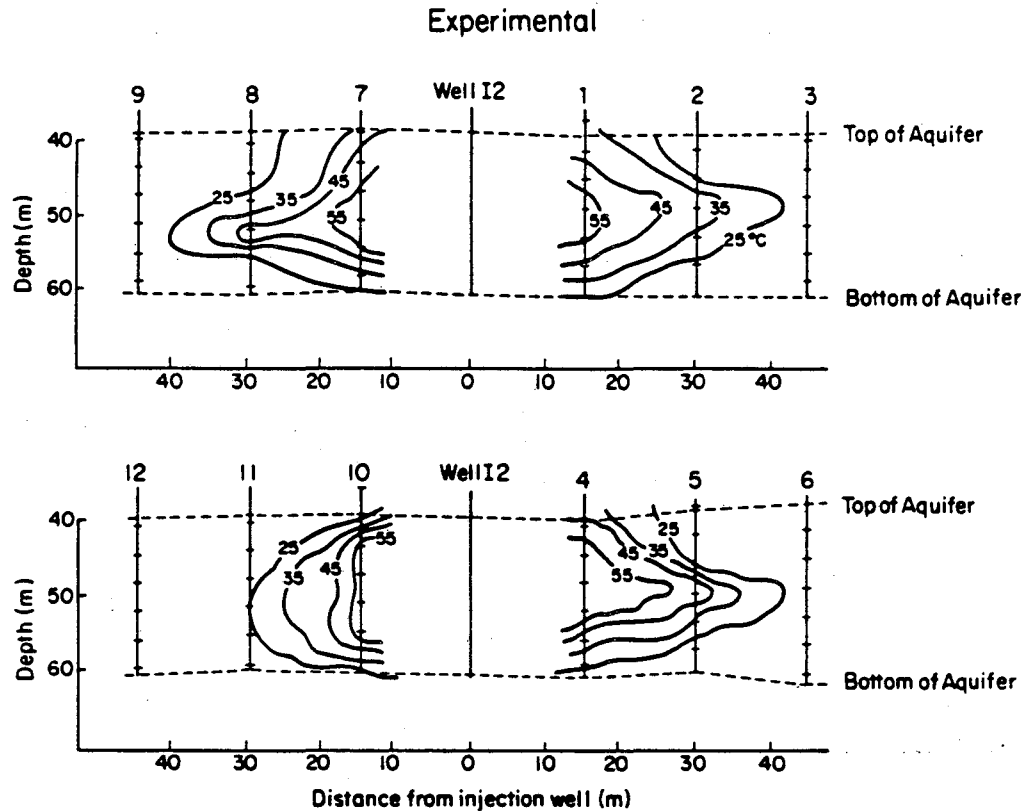
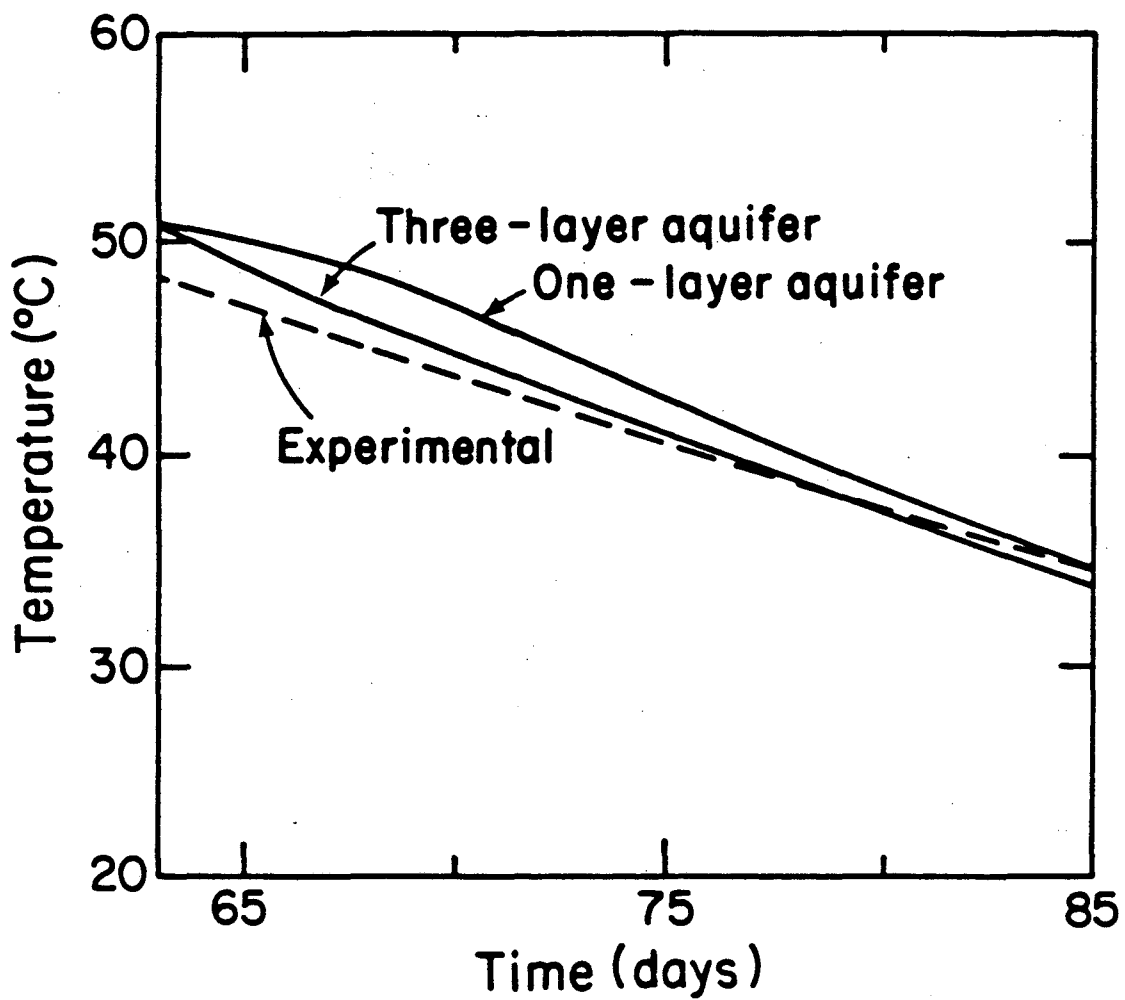


Fig. 5. Temperature profiles illustrating mesh variation.



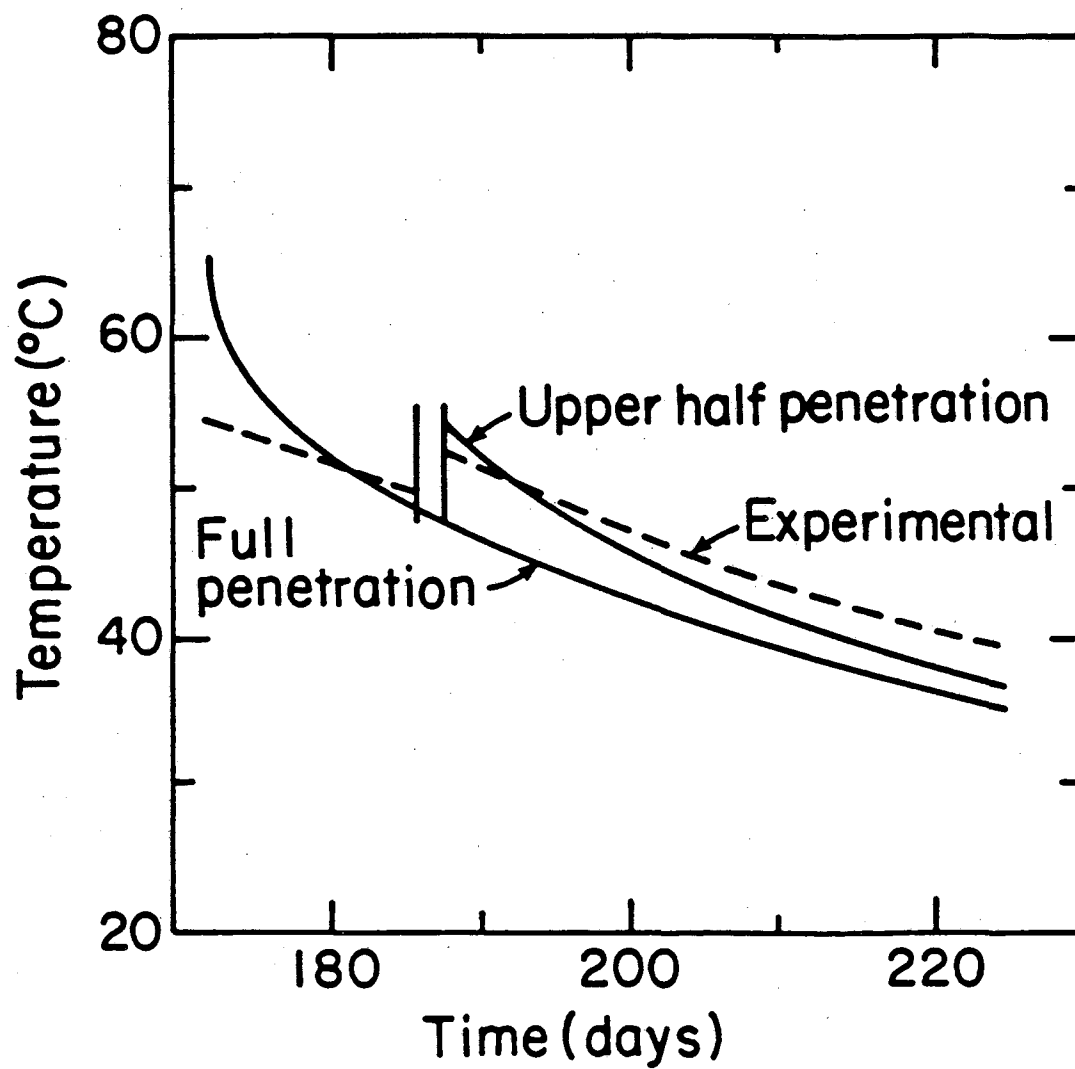
XBL 8412-5401

Fig. 6. Temperature contours after the third-cycle injection period.



XBL 8412-6199

Fig. 7. Third-cycle production temperature.



XBL 8211-2688

Fig. 8. Fourth-cycle production temperature.

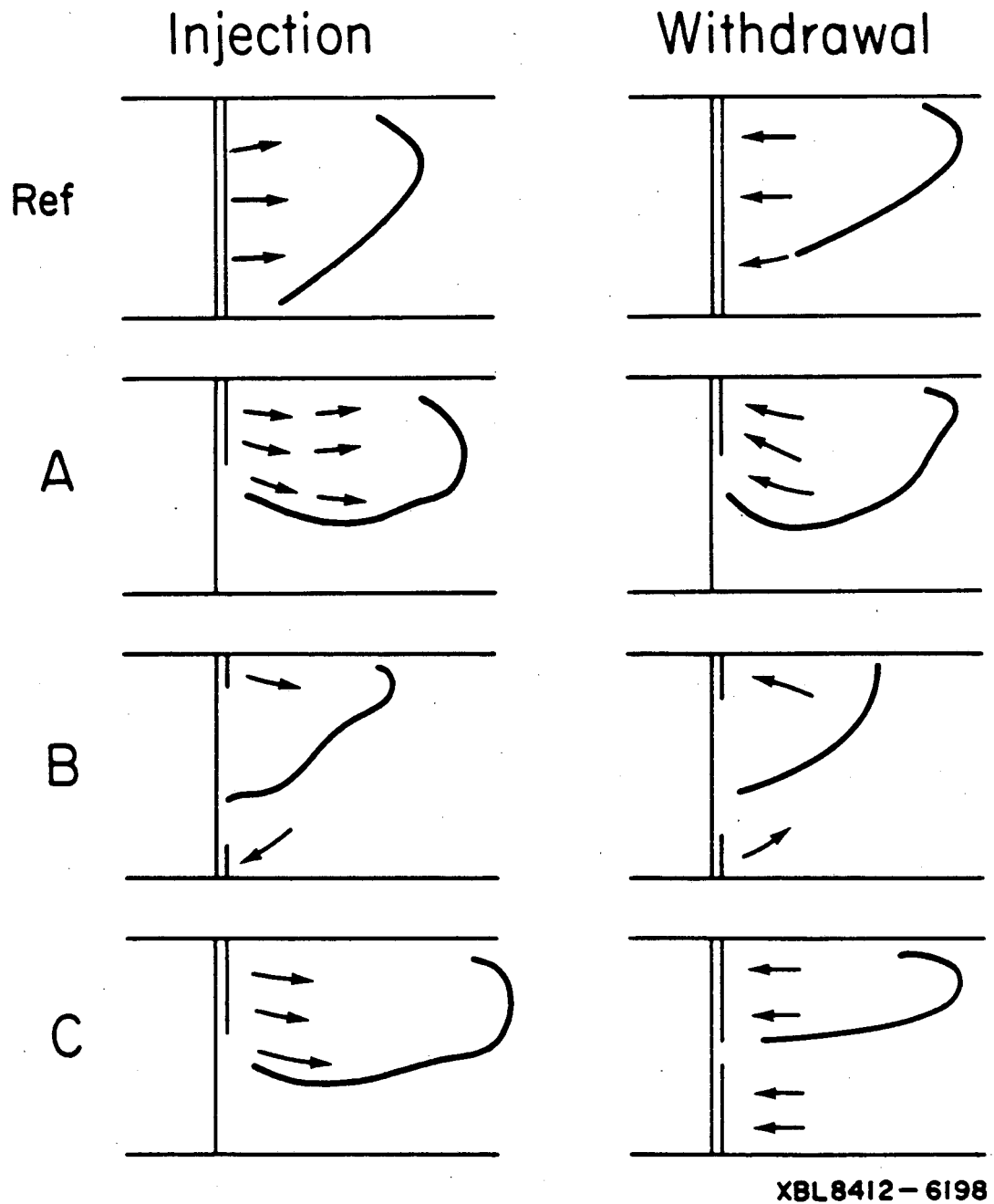
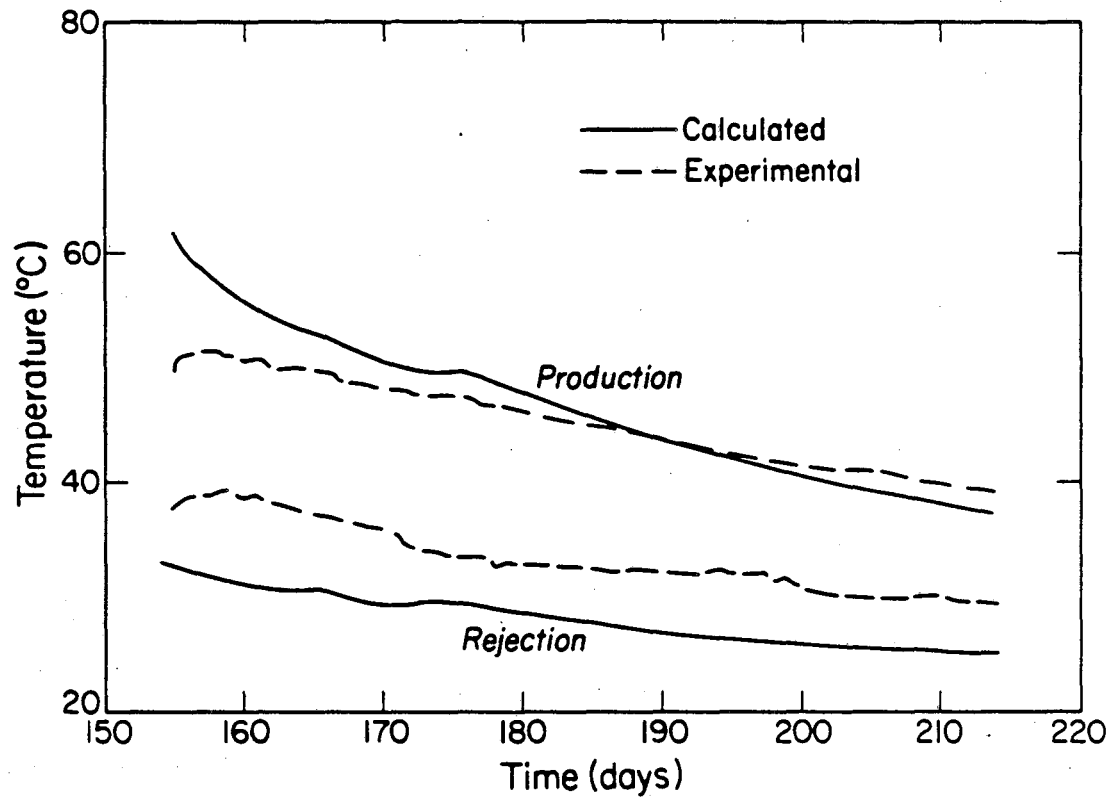


Fig. 9. Schematic diagram showing design-study alternatives.



XBL 8412-6196

Fig. 10. Fifth-cycle production temperature.

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TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720