Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

Presented at the International Conference on Subsurface Heat Storage in Theory and Practice, Stockholm, Sweden, June 6-8, 1983

AQUIFER STORAGE SIMULATION - IN THEORY AND IN PRACTICE

C.F. Tsang

June 1983

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

DISCLAIMER

Presented at the International Conference on Subsurface Heat Storage in Theory and Practice, Stockholm, Sweden, June 6-8, 1983.

AQUIFER STORAGE SIMULATION - IN THEORY AND IN PRACTICE

Chin Fu Tsang

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

June 1983

ABSTRACT

The paper reviews the various uses of simulation studies by means of mathematical modeling in the area of aquifer thermal energy storage. A discussion is given of the governing equations and the key elements and alternative assumptions that enter into these equations. A numerical model used by Lawrence Berkeley Laboratory is then described and its validation discussed. Recent applications of this model to make a priori predictions of a series of field experiments are then presented. Thus this paper attempts to summarize the aquifer energy storage simulation studies from theory to practice.

INTRODUCTION

In the study of thermal energy storage in aquifers, simulation studies with mathematical models play an important role. Their uses may be listed as follows:

1. To understand key processes. By generic studies, isolated key factors can be investigated and an understanding of the processes obtained. These key factors may be, for example: thermal front tilting, thermal dispersion, etc.

2. To determine sensitivity to key parameters. This will help to set requirements for how accurately a parameter should be measured in the field or in the laboratory.

3. As an experiment design tool. By using modeling, crucial guidelines concerning field experiment layout and the required instrumentation sensitivity can be determined.

4. As a test against field data. Any discrepancy will either point out some error and inaccuracy in the model, or, more interestingly, uncover unexpected processes or effects not yet built into the model.

5. As a prediction tool. By simulation using site-specific conditions, predictions can be made for different scenarios or for later times.

In the paper we shall first give a discussion of the governing equations that form the basis of the mathematical modeling and the key elements and alternative assumptions that enter into these governing equations; then a number of solution methods will be briefly described. A numerical model used by Lawrence Berkeley Laboratory (LBL) in the aquifer energy storage studies will be introduced and its recent application to the 1981-1982 field experiment carried out at the Mobile site by Auburn University will be discussed. Thus this paper attempts to review the aquifer energy storage simulation studies from theory to practice.

GOVERNING EQUATIONS

The state of hot or cold water flowing through a porous medium can be described by the velocity $\bar{v}$ and any two thermodynamic quantities pertaining to the fluid--for instance, the pressure P and the temperature T. In the continuum approximations used to model average behavior, the microscopic velocity $\bar{v}$ within individual fractures or pores is related to the macroscopic velocity $\bar{q}$ averaged over the rock mass by $\bar{v} = \bar{q}/\phi$, where ϕ is the porosity. In most thermohydrologic models, the velocity is a derived quantity determined by the pressure and temperature distributions. The equations governing pressure and temperature are based on mass and energy conservation laws. The choice of pressure and temperature as variables describing the state of a fluid is arbitrary. All thermodynamic quantities are determined by the values of any two of them, together with the equation of state. Density, ρ^w, internal energy U, enthalpy H, and others can also be used to determine the state of fluid flow and heat transfer.

Fluid Velocity

The flux of fluid $\bar{q}$ flowing relative to the solid rock is determined by the permeability of the formation $\bar{\bar{k}}$, the viscosity of the fluid μ, and the driving forces of pressure gradient ∇P and gravitational body force $\rho^w \bar{g}$:

$$\bar{q} = -\frac{\bar{\bar{k}}}{\mu} (\nabla P - \rho^w \bar{g}).$$

This is the familiar Darcy's law for the equation of motion. Darcy's law is an approximation of the general Navier-Stokes equation for momentum conservation. Permeability $\bar{\bar{k}}$ is one of the most important hydraulic properties of the formation.

Different approximations commonly used for the treatment of permeability are: (a) the permeability is independent of the variables (pressure, temperature, stress, etc.) and is treated as an input parameter for each grid block; (b) the permeability is a function of pressure and temperature, k(P,T). This is usually assumed for a fractured medium. The permeability-temperature dependence may also be important to take into account the effects of thermal stress and thermally induced rock-fluid interactions; (c) the permeability is also a function of stress, $k(\bar{\sigma})$. In addition to the pressure and temperature field, the tensor stress field is modeled. The stress changes may be induced by hydraulic, mechanical, or thermal loading.

The fluid velocity is inversely proportional to the dynamic viscosity μ. The usual approximations for μ in the different models are: (a) the viscosity is a constant. This is the case for isothermal saturated flow; (b) the viscosity is a function of temperature $\mu(T)$. Most of the nonisothermal saturated flow models use formulas or tables to account for this dependence. (c) Under two-phase (e.g., steam-water) conditions, the effects of viscosity are modified by the relative permeabilities, which are mainly functions of fluid saturation S.

The fluid flow is proportional to the driving force or gradient. The usual approximations used are: (a) the variation in the gravitational force $\rho^w \bar{g}$ is neglected. This is a good approximation for slightly compressible flow when the liquid density variation with pressure is small. (b) The Boussinesq approximation is used for the gravitational force imbalance (buoyancy) between hot and cold water. The density variation with temperature is considered only in the buoyancy force and is neglected in other terms of the governing equations. (c) The driving forces are the pressure gradient and the gravitational body force, $\nabla P - \rho^w \bar{g}$, for nonisothermal, saturated flow. (d) For two-phase flow, the density of liquid and the density of vapor are different. The driving force for each phase is $\nabla P - \rho^\alpha \bar{g}$, $\alpha = \ell, v$. Both phases are assumed either to have equal pressure, or different pressures if the capillary pressure is taken into account.

Fluid Flow Equation

The governing equation for the fluid flow is based on the conservation of fluid mass, or equivalently, the balance of the rate of change, the flux, and the prescribed source/sink of fluid mass:

$$\frac{\partial(\phi\rho^w)}{\partial t} + \nabla \cdot (\rho^w \bar{q}) = Q_F.$$

This equation of continuity, combined with Darcy's equation for $\bar{q}$, determines the pressure field. The variation of the porosity of the formation and the variation of the density of the fluid determine the transient term $\partial(\phi\rho^w)/\partial t$. The approximations usually used are: (a) $\Delta\phi = 0$ for constant porosity; (b) $\Delta\phi$ is linear in pressure change; (c) ρ^w is slightly compressible with pressure increase and expandable with temperature increase; (d) ρ^w is a nonlinear function of pressure and temperature; and (e) for a liquid-vapor mixture, the density is $\rho = S^\ell\rho^\ell + S^v\rho^v$, with the saturations related by $S^\ell + S^v = 1$. Steam tables or nonlinear formulas are required to evaluate the sensitive changes of density.

Heat Transfer Equation

The governing equation for the heat transfer through the formation is based on the conservation of energy:

$$\frac{\partial(\rho^m U)}{\partial t} + \nabla \cdot (\rho^w \bar{q} H) - \nabla \cdot (\bar{\bar{K}}_H \cdot \nabla T) = Q_H.$$

The conservation of energy is expressed in terms of the rate of change of internal energy U of the fluid-rock mixture, the convective flux of enthalpy H of the fluid, the diffusive flux (conduction and/or dispersion) driven by the temperature gradient, and the heat source/sink Q_H. For single-phase models, the thermodynamic functions U and H are usually expressed in terms of temperature and/or pressure. Under two-phase conditions, steam tables or formulas are required to evaluate the nonlinear changes of U and H, together with the density ρ and other fluid properties. Some of the two-phase models use U or H as a primary variable.

For the transient internal energy accumulation term, $\partial(\rho^m U)/\partial t$, the different expressions used in the various studies are: (a) $C_H^m(\partial T/\partial t)$, with a constant bulk heat capacity C_H^m ($= \rho^m c^m$) for the fluid-rock mixture; (b) $[\phi\rho^w c^w + (1 - \phi)\rho^r c^r](\partial T/\partial t)$, where $\rho^w c^w$ is the heat capacity of fluid and $\rho^r c^r$ is the heat capacity of the rock; (c) $(\partial/\partial t)[\phi\rho H + (1 - \phi)\rho^r c^r T] - (\partial/\partial t)(\phi P) = (\partial/\partial t)[\phi S^\ell\rho^\ell H^\ell + \phi S^v\rho^v H^v + (1 - \phi)\rho^r c^r T]$ for two-phase flow. The enthalpy H is related to the internal energy U by the definition $H = U + P/\rho$. The pressure term due to compressible work is usually neglected in the two-phase energy equation.

The convective flux term can be expressed as: (a) $C_H^w \bar{q} \cdot \nabla T$ or $\rho^w c^w \bar{q} \cdot \nabla T$, where C_H^w or $\rho^w c^w$ is the heat capacity of the fluid. The heat is carried by the fluid with velocity $\bar{q}$; (b) $\nabla \cdot (\rho^w \bar{q} H)$ for saturated flow; (c) $\nabla \cdot (\rho^\ell \bar{q}^\ell U^\ell + \rho^v \bar{q}^v U^v)$ for two-phase flow with the pressure work neglected.

The diffusive flux is usually approximated by: (a) $\nabla \cdot K_T \nabla T$ for isotropic conduction with a scalar thermal conductivity K_T; (b) $\nabla \cdot (\bar{\bar{K}}_T \cdot \nabla T)$ for anisotropic conduction with a tensorial thermal conductivcity $\bar{\bar{K}}_T$; and (c) $\nabla \cdot ((\bar{\bar{K}}_T + \bar{\bar{K}}_{TD}) \cdot \nabla T)$ for both conduction and dispersion through the formation. The thermal dispersion depends on the fluctuations of microscopic velocities. The dispersive contribution can be regarded as an enhancement to heat conduction in the presence of fluid movement. Usually a

linear relationship is assumed between the components of the dispersivity $\bar{\bar{K}}_{TD}$ and the components of the microscopic velocity $\bar{v} = \bar{q}\phi$.

Coupling of Fluid Flow and Heat Transfer

The fluid flow equation and the heat transfer equation are coupled through the fluid velocity $\bar{q}$ in the flux terms and through the temperature and pressure dependences of the fluid properties (ρ^w, μ) and formation properties (k, ϕ). In most models using Darcy's approximation, the flow velocity equation is substituted into the fluid flow equation and the heat transfer equation. The elimination of $\bar{q}$ simplifies the set of governing equations for thermohydrologic flow to two equations for the pressure and temperature fields. Once these fields are determined, the Darcy velocity $\bar{q}$ or the microscopic fluid velocity $\bar{v}$ is calculated from the pressure gradient, buoyancy force, viscosity, and permeability.

ANALYTICAL AND NUMERICAL SOLUTIONS

Unless drastic simplifying assumptions can be made, the governing equations described above cannot be solved by analytic methods. Semi-analytic approaches have been suggested whose applications are limited in scope, dependent on the particular simplifications assumed. An example is the "Steady-Flow Model," which assumes a steady radial fluid flow field (Doughty et al., 1982). Thus convection around a single injection-production well is simulated by translating the temperature field in steps according to the steady flow field on an equal-volume finite-difference radial mesh. The mesh is designed to minimize numerical dispersion. The aquifer is assumed to be homogeneous and horizontal, the cap and bedrock impermeable, and all material properties temperature-independent. This simple model has been applied successfully to problems where buoyancy flow may be neglected, and, based on this, a graphical method of analyzing aquifer thermal energy storage performance has been proposed (Doughty et al., 1982).

In general, even for rather simple problems involving uniform aquifer properties, numerical solution of the coupled governing equations is needed. Three numerical methods are usually used: (1) finite-difference, (2) integrated-finite-difference, and (3) finite-element. Each has its own strengths and areas of optimal applications.

A numerical model that LBL has been using for our simulation studies of aquifer thermal energy storage over the last few years is called PT. This is an improved version of the program CCC, with a new mathematical formulation and an advanced matrix solution scheme. It uses the integrated-finite-difference numerical technique to compute the heat and fluid flow in a liquid-saturated porous medium. One-dimensional consolidation of the system can also be simulated. In this program, both the permeability and the viscosity may be temperature-dependent. Density of the fluid is temperature- and pressure-dependent through an equation of state, and the gravitational body force is taken into account. The capability to calculate anisotropic conduction and convection with different thermal conductivities and hydraulic conductivities along the major axes of the mesh is included in the program.

PT has been validated against a number of analytical and semi-analytical solutions for fluid and heat flow. These are listed below:

1. Continuous Line Source (Theis, 1935).

2. Cold Water Injection in a Hot Reservoir (Avdonin, 1964).

3. The temperature variations at a production well due to cold water injection (Gringarten and Sauty, 1975).

4. Conduction Problem (Carslaw and Jaeger, 1959).

5. Two-Node Problem: Transient conduction heat transfer between two nodes.

6. The rate of thermal front tilting when hot water is injected into a cold reservoir(Hellstrom et al., 1979).

7. The pressure response in a well intercepting a finite conductivity vertical fracture (Cinco-Ley et al., 1978).

8. The pressure response in a well intercepting an infinite conductivity horizontal fracture (Gringarten, 1971).

PT has also been validated against a series of field experiments. Numerical modeling of two cycles of injection, storage, and production of hot water in a confined aquifer yielded results that closely matched temperatures, pressures, and energy recovery factors observed in the field (Tsang et al., 1979). Details and sources of the validation solutions may be found in Mangold et al. (1980).

RECENT APPLICATION OF SIMULATION STUDIES TO AUBURN UNIVERSITY FIELD EXPERIMENTS CARRIED OUT DURING 1981-1982

During 1981 and 1982, Auburn University performed a three-cycle aquifer thermal energy storage field experiment in Mobile County, Alabama (Molz et al., 1983). Concurrent with the first two cycles (59°C and 82°C), Lawrence Berkeley Laboratory (LBL) did numerical simulations based on field operating conditions to predict the outcome of each cycle before its conclusion. Prior to the third cycle, a series of numerical simulations were made to aid in the design of an experiment that would yield the highest recovery factor possible.

First-Cycle Prediction

During the first cycle, 25,000 m^3 of water at an average temperature of 59°C was injected over a period of one month into a 21 m-thick aquifer. It was then stored for one month and subsequently produced. The injected water was obtained from a supply well perforated in the same aquifer 240 m away from the injection/production well. LBL was provided with the basic geological, well test, injection flow rate and injection temperature data, as well as the planned production flow rate.

Table 1. Parameters used in the first-cycle prediction numerical simulation.

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
Aquifer horizontal permeability	63 darcies
Aquifer vertical to horizontal permeability ratio	1:7
Aquitard to aquifer permeability ratio	10^{-5}
Porosity	
Aquifer	0.25
Aquitard	0.35
Storativity	
Aquifer	6×10^{-4}
Aquitard	9×10^{-2}

The well-test data and geological information were studied and analyzed to obtain reservoir parameters and their range of uncertainty. The parameters used in our numerical simulation are listed in Table 1. Since the supply well is 240 m from the injection/production well and the thermal radius was calculated to extend only about 25 m, it was decided that a radial calculation mesh would be adequate. Based on the flow rates and injection temperature provided, we simulated the experiment using the numerical model PT. The calculated production temperature is presented as curve A in Figure 1, where the experimental result is also plotted. The experimental results were made known to us after we completed and presented our results. The predicted energy recovery factor is 0.61 compared to the experimental value of 0.55. This agreement is satisfactory.

First Cycle: Detailed Comparison between Theory and Experiment

A series of parameter studies were also made comparing the experimental and calculated temperature fields at various times during the first cycle. These studies led us to hypothesize that the aquifer is vertically stratified into three layers, the middle layer (5 m thick) having a permeability 2.5 times that of the upper and lower layers. Using this model, the first-cycle recovery factor was calculated to be 0.58, calculated production temperature is shown as curve B in Figure 1. Apparently the layered structure of the aquifer noticeably lowers the recovery factor. This is significant because layering is usually not obtained through conventional well-test analysis.

Second-Cycle Prediction

The procedure was similar to the first-cycle prediction. Only the injection flow rate, temperature history, storage period, and expected average production flow rate were made known to us. The three-layered aquifer model described in the previous section was used for the calculation. Water at an average temperature of 82°C was injected over a period of about 4.5 months. The variable, experimental injection flow rates and temperatures were averaged into five segments for the numerical simulation. The

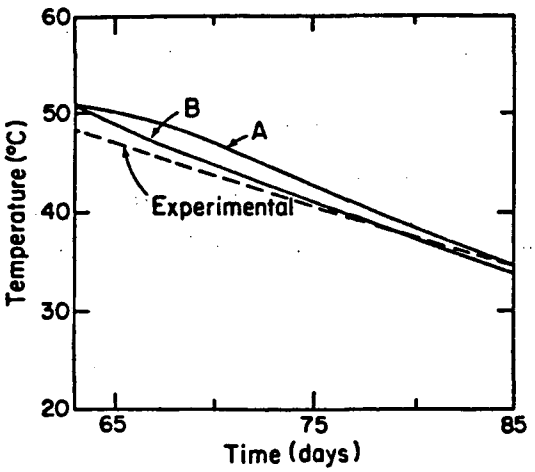

Figure 1. First-cycle production temperature.

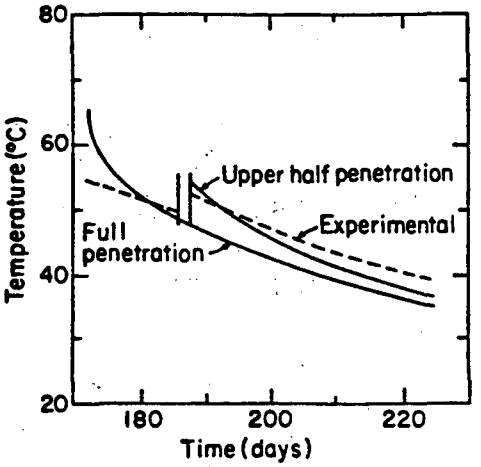

Figure 2. Second-cycle production temperature

total volume injected, about 58,000 m^3, was considerably larger than the volume injected during the first cycle; hence the thermal radius extended farther than in the first cycle (to about 38 m). However, this distance is still small enough compared to the distance to the supply well to justify using a radial calculation mesh. After injection, the hot water was stored for 34 days.

The simulation of the original production plan--to produce all the injected water through the fully penetrating well screen that had been used throughout the experiment--was carried out, using a constant fluid flow rate of 200 gpm. The calculated recovery factor is 0.40 and the production temperature is shown in Figure 2.

However, this production plan was changed after two weeks of production. At that time the well was shut down and modified to produce fluid from only the upper half of the aquifer; then production was resumed. This scenario was again simulated using a constant flow rate of 200 gpm. The calculated recovery factor is 0.42; the production temperature is shown in Figure 2. After the second-cycle calculation was completed the experimental results were made known to us: the recovery factor is 0.45, and the production temperature is shown in Figure 2. Comparisons between the experimental and calculated temperature fields in the aquifer throughout the second cycle show acceptable agreement.

Third-Cycle Design Studies

Simulation studies were also used in the planning for the third-cycle experiment. Alternative injection and production schemes were studied to maximize the recovery factor for a three-month cycle with constant injection flow rate of 112 gpm and temperature of 82°C. Making use of the knowledge gained from the first- and second-cycle simulations, that buoyancy flow is strong, three approaches were taken. These are shown schematically in Figure 3, along with a reference case that uses full penetration during injection and production. These three approaches are explained as follows:

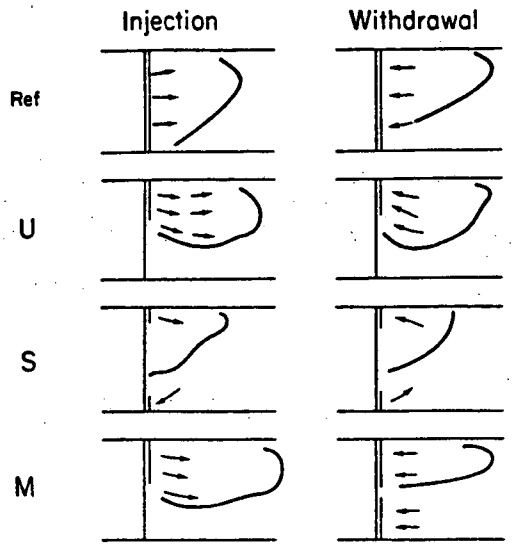

Figure 3. Schematic drawing of different injection-withdrawal schemes.

1. 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 (labeled U).

2. "Modified SPEOS." 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 (labeled S).

3. 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. In this way the colder water will not be pulled into the upper well where it would lower production temperature (labeled M).

Table 2 summarizes the results of the numerical simulations. From this table we find that the maximum recovery factor obtained among all the cases studied is 0.52, representing an improvement of about 25 percent over the reference case.

Table 2. Third-cycle Design Studies. T = 82°C, Q = 112 gpm; 1 month each of injection, storage, and production.

Case	Well Screen Interval		ε
	Injection	Production	
Ref.	Full	Full	0.40
U1	Upper 40%	Upper 40%	0.45
U2	Upper 40%	Upper 20%	0.50
S1	Upper 20% Lower 20%	Upper 20%	0.52
S2	Upper 20% Lower 20%	Upper 20% Lower 20%	0.49
M1	Upper 40%	Upper 40% Lower 55%	0.50
M2	Upper 40%	Upper 20% Lower 55%	0.52

CONCLUSIONS

The theory of heat and fluid flow and the key parameters involved are reviewed in regard to the application to simulation of aquifer thermal energy storage. The successful prediction of the first- and second-cycle energy recovery factors, based on the numerical model PT, has demonstrated that the main physical processes occurring in the Mobile field are probably well understood and can be properly simulated by the numerical model PT. The third-cycle design studies consider a substantial number of alternative injection/production schemes. Results have been transmitted to Auburn University for consideration in their decisions concerning the third-cycle experiment. This demonstrates the value of numerical modeling. If one were to experimentally carry out all the alternative designs, an order of magnitude increase in budget and time would be required.

ACKNOWLEDGEMENTS

Continual assistance and cooperation from my colleagues, C. Doughty and J. S. Y. Wang is much appreciated. This work was supported by the Assistant Secretary of Conservation and Solar Energy, Office of Advanced Conservation Technology, Division of Thermal and Mechanical Storage Systems of the U. S. Department of Energy under Contract DE-AC03-76SF00098. This report represents work performed within the Seasonal Thermal Energy Storage Program managed by Pacific Northwest Laboratory.

REFERENCES

Doughty, C., Hellstrom, G., Tsang, C. F., and Claesson, J., 1982. A dimensionless-parameter approach to the thermal behavior of an aquifer thermal energy storage system. Water Resources Research, v. 18, no. 3, p. 571-587.

Mangold, D. C., Lippmann, M. J., and Bodvarsson, G. S., 1980. Computer program CCC/PT user's manual, version II. Lawrence Berkeley Laboratory report LBL-10909, Berkeley, California 94720.

Molz, F. J., Melville, J. G., Parr, A. D., King, D. A., and Hopf, M. T., 1983. Aquifer thermal energy storage: A well doublet experiment at increased temperatures. To be published in Water Resources Research.

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.

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