Final Report for
"Hydrologic Studies Support"
INTERCOMP Code Conversion

Vernon Ichimura

DEPARTMENT OF CIVIL AND ENVIRONMENTAL ENGINEERING

COLLEGE OF ENGINEERING

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FINAL REPORT FOR "HYDROLOGIC STUDIES SUPPORT":

INTERCOMP CODE CONVERSION

by

Vernon Ichimura

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ABSTRACT

Mass and energy balance errors noted in a number of IBM-executed problems are caused by the lack of precision in computing total mass and energy values for a domain. This problem is evident in domains constructed with highly variable mesh sizes during the early time of simulation. The machine round-off was corrected by double-precisioning certain calculations for mass and energy balance.

Small differences that exist between the improved INTERCOMP code operating on an IBM machine and the "old" version on a CDC machine seem unimportant. The noted differences are greatest at an onset of physical system perturbation. These differences diminish rapidly with each succeeding time step.

Comparisons with numerical and analytical solutions appear to prove authenticity of code results. Numerical comparisons with the CCC computer code on the Mobile experiment data demonstrate the advantage of using aquifer influence functions in place of an infinitely large mesh. The one-dimensional heat transfer in the overburden and underburden appears sufficiently accurate to describe aquifer heat losses.

TABLE OF CONTENTS

	Page
ACKNOWLEDGMENTS	ii
ABSTRACT	iii
LIST OF TABLES	viii
LIST OF ILLUSTRATIONS	ix
INTRODUCTION	1

PART 1

NOMENCLATURE

PART 1	4
Units	4
Upper Case Roman Letters	5
Lower Case Roman Letters	7
Greek Letters	9
Functions	9
Subscripts	9
Superscripts	10

PART 2

TECHNICAL INFORMATION ON INTERCOMP CODE

PART 2	13
INTRODUCTION	13
RESERVOIR MODEL	14
RESERVOIR EQUATIONS	15
DENSITY MODEL	21
VISCOSITY MODEL	23
ENTHALPY MODEL	27

FINITE DIFFERENCE SOLUTION METHOD	32
INITIAL AND BOUNDARY CONDITIONS	45
WELLBORE MODEL	52
PROGRAM STRUCTURE	58
MAIN PROGRAM	59
SUBROUTINES	63
SELECTION OF SOLUTION, GRID, AND TIME STEP SIZE	73
SUMMARY	78

PART 3

PROBLEM STATEMENT

PART 3	82
INTRODUCTION	82
TEST RADIAL COORDINATE PROBLEM	83
CODE COMPARISON RESULTS	97
MISCELLANEOUS CHANGES	106

PART 4

SOLUTION COMPARISONS

PART 4	109
INTRODUCTION	109
THEIS SOLUTION	110
SHAPE TEST PROBLEM	113
HOOPES AND HARLEMAN PROBLEM	121
ONE DIMENSION TEST	127
AVDONIN PROBLEM	133
GRINGARTEN AND SAUTY SOLUTION	143

PART 5AUBURN UNIVERSITY FIELD EXPERIMENT

PART 5	153
INTRODUCTION	153
EXPERIMENT AND SIMULATION	153

PART 6DISCUSSION AND CONCLUSIONS

PART 6	185
CODE CHANGES	185
CODE PHYSICAL INPUT PARAMETERS	186
MODEL CONSTRUCTION AND OPTION DATA	189
CONCLUSION	194

APPENDIX

A. TAPE DOCUMENTATION	199
B. EQUATION DERIVATION DETAILS	206
HEAT LOSS TO OVERBURDEN AND UNDERBURDEN	206
WELLBORE HEAT TRANSMISSION	212
C. BOUNDARY CONDITIONS RELATED PARAMETERS	217
INTRODUCTION	217
WELLBORE DATA	218
WELLBORE MODEL SPECIFICATION OPTIONS	221
AQUIFER INFLUENCE FUNCTIONS	230
Carter-Tracy	231
Pot Aquifer	236
Steady-State Aquifer	238

D. USERS INSTRUCTIONS	241
CHANGES IN THE NOMENCLATURE	241
REDIMENSIONING THE PROGRAM	241
INPUT DATA CARDS	243

LIST OF TABLESPART 2

Table	Page
2-1 Enthalpy of Saturated Water	29
2-2 Compressed Water Enthalpy	30
2-3 Summary of Numerical Diffusion and Stability	78

PART 3

3-1 Computer Data Characteristics	83
3-2 Radial Test Problem Physical Data	87

PART 4

4-1 Physical Data for Theis Solution Comparison	113
4-2 Physical Data for Shape Test	121
4-3 Physical Data for Hoopes and Harleman Solution	127
4-4 Physical Data for One-dimensional Linear Solution	130
4-5 Physical Data for Avdonin Solution	142
4-6 Physical Data for Gringarten and Sauty Problem	150

PART 5

5-1 Physical Data for the Mobile Experiment	165
5-2 Energy Budget	170

PART 6

6-1 Flow Allocation Comparisons	193
---	-----

APPENDIX A

A-1. Tape Library	199
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APPENDIX C

C-1. Summary of Well Specification Options	229
C-2. Carter Tracy Limited Aquifer Functions	235

LIST OF ILLUSTRATIONS

PART 2

Figure	Page
2-1 Generalized reservoir finite difference molecule.	36
2-2 Temperature assignments to overburden and underburden blocks.	51
2-3 Wellbore data definition. Part A shows input data definitions and solution increments, and part B is a section of a generalized wellbore consisting of the inner tubing and outer casing.	54
2-4 Operating structure of the INTERCOMP DWDM. MAIN program serves as the operating skeleton for the DWDM. (Modified from figure 2 in INTERCOMP, 1976).	62
2-5 Solution scheme arrangement in subroutine [ITER]. (Modified from INTERCOMP, 1976).	67
2-6 Locations of transmissibility T relative to grid block transmissibility tables printed by [PRINTS].	72
2-7 Schematic of the simulator (adapted from INTERCOMP, 1976).	80

PART 3

3-1 Schematic of test comparison problem. Aquifer zone is anisotropic and inhomogeneous 10 x 1 x 5 (x,y,z) finite difference grid.	86
3-2 Energy balance on variable grid size problem.	91
3-3 Energy balance comparisons using REAL*4 and REAL*8 arrays.	95
3-4 Energy balance on a problem of uniform grid size.	96
3-5 Comparison of maximum grid block δp results from the direct solver algorithm in the DWDM. The small graph shows the magnitude of relative difference between δp values.	101
3-6 Comparison of the solver output of maximum change in temperature (δT) between IBM and CDC results. The small graph shows the relative differences between the IBM and CDC results.	102
3-7 Heat loss calculation differences for IBM and CDC in an identical problem. The heat loss calculations by CDC (circles) are higher than IBM (squares).	103

3-8	Fluid efflux across the outer boundary comparisons.	104
3-9	Comparison of energy efflux at the periphery boundary.	105

PART 4

4-1	Theis analytical solution comparison	112
4-2	Reservoir schematic for shape test problem. Reduced permeability region is shown shaded.	116
4-3	Element to parent element relationship and numbering scheme. . .	117
4-4	Dimensionless pressure distribution comparisons for an isotropic flow field.	119
4-5	Dimensionless pressure distribution comparisons for an anisotropic flow field.	120
4-6	Hoopes and Harleman solution comparison.	125
4-7	Solute concentration comparison to Hoopes and Harleman analytical solution.	126
4-8	One dimensional temperature solution comparisons. Length equal to 1.0 is the same as 198.12m (650 ft).	131
4-9	Solute concentration solution comparisons. Length equal to 1.0 corresponds to 381.00m (1250 ft).	132
4-10	Radial Avdonin problem comparisons. Maximum dimensionless radius corresponds to 15.24m (50 ft).	138
4-11	Radial Avdonin problem compared to a cartesian coordinate approximation solution. Maximum radius of 1.0 corresponds to 15.25m (50 ft).	139
4-12	One-dimension linear Avdonin solution comparison results. Dimensionless length of 1.0 corresponds to 30.48m (100 ft). . .	140
4-13	One-dimension linear Avdonin solution comparison results with extended overburden boundaries and higher node density. Dimensionless length of 1.0 corresponds to 30.48m (100 ft). . .	141
4-14	Nomenclature for an arbitrary stream channel. The variable A is a dimensionless area.	147
4-15	Comparison of the Gringarten and Sauty problem with INTERCOMP results. (Continuous results are adapted from Gringarten and Sauty, 1975, figure 6).	148

4-16	Areal map of temperature distribution at time = 500 days for $\lambda = 6.00$	149
------	--	-----

PART 5

5-1	Plan view of the Mobile ATES experiment well field. Injection well 2 is used for this experiment.	159
5-2	Sectional schematic of the Mobile Experiment (Adapted from Moltz, et al., 1980).	160
5-3	Finite difference radial mesh for the Mobile experiment simulation.	161
5-4	Injection rate and temperature for first cycle simulation. . . .	162
5-5	Injection rate and temperature for second cycle simulation. . . .	163
5-6	Production rates for cycles one and two.	164
5-7	Simulation comparisons for 9 meters (29 ft) radial distance at thermistor B.	173
5-8	Simulation comparisons for 18 meters (59 ft) radial distance at thermistor B.	174
5-9	Simulation comparisons for 21 meters (69 ft) radial distance at thermistor B.	175
5-10	Simulation comparisons for 37 meters (121 ft) radial distance at thermistor B.	176
5-11	Comparisons for simulation at 45 meters (148 ft).	177
5-12	Production temperature comparisons during the first cycle. . . .	178
5-13	Production temperature comparisons during the second cycle. The arrow signifies time at which the second cycle efficiency is computed.	179
5-14	Temperature contour comparisons between LBL, INTERCOMP and observed results. The time is 129.73 days, at the end of storage in the first cycle.	180
5-15	Temperature contour comparisons at the end of simulation of first cycle. Time is 170.83 days.	181
5-16	Temperature contour comparisons at the end of injection for the second cycle. Time is 63.38 days after the start of second cycle.	182

5-17 Temperature contour comparisons after production in the second cycle. Time is 181.30 days since the beginning of second cycle of simulation	183
--	-----

APPENDIX B

B-1. Finite difference block schematic for overburden layers.	208
B-2. Diagram of a wellbore.	214

APPENDIX C

C-1. Schematic of a wellbore in radial coordinates.	219
C-2. Test of aquifer influence functions, at an observation well located at $r = 45$ ft. (Adapted from Figure 10 in INTERCOMP, 1976). . .	240

APPENDIX D

D-1. Diagram of initial parameters.	253
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INTRODUCTION

The INTERCOMP Deep Well Disposal Model (DWDM) (INTERCOMP, 1976) was set up at Washington State University (WSU) as part of an earlier feasibility study of an Aquifer Thermal Energy Storage (ATES) demonstration project at Bellingham, Washington, where initial plans called for the use of the code as a design and management tool. A more recent request for proposals for ATES projects resulted in a number of proposed demonstration project plans calling for extensive use of the DWDM; however, because of changes in funding a number of these projects are being phased out.

A preliminary study of a test-case example documented in the DWDM manual (INTERCOMP, 1976) showed poor mass and energy balance output, suggesting that machine round-off is occurring in the code when it is run on an International Business Machine (IBM) type computer. This problem was not found when the same input was submitted to a Control Data Corporation (CDC) machine. Similar perfect mass and energy balance were obtained when the test problem was submitted on an IBM with the code modified with fully double-precision real variables. Because of the proposed extensive use of the code, the accessibility of IBM-type machines, and the availability of funds, this project was allowed to continue.

The INTERCOMP code was first released in 1976 for the purpose of simulating the behavior of liquid wastes injected in deep saline aquifers (version one). Newer versions released by the former INTERCOMP subsidiary INTERA Environmental Consultants, Inc., are now available. Version two, released in 1977

(INTERA, 1977), was designed to simulate migration of multiple components of trace radionuclides from a breached geologic repository; this was in addition to the capabilities available version one. A third version, released in 1979 (INTERA, 1979), is similar to version one with new options which include single component contaminant decay and adsorption, a free surface option limited to the uppermost grid blocks, and allowance for surface recharge. Additional revisions of the three codes are continuing at INTERA and newer, more efficient versions are expected in the near future. Version two is known to exhibit computational difficulties when run on a Sperry UNIVAC or similar machines for simulating radionuclide transport.

The purpose of this report is to modify and correct the code for the above-mentioned problem and to verify code responses by comparing output results to known analytical and simple numerical solutions. In addition, results from the Mobile ATEs research project and simulation by the Lawrence Berkeley Laboratory CCC computer code (Tsang, Buscheck, and Doughty, 1981) are compared to results obtained by the INTERCOMP code using similar input data.

Theory and code format are given for completeness. Emphasis is given to the heat transfer aspect and to areas that are unclear in the original document. References to actual code variables are used to acquaint the user with some of the more important code variables. Dimensions are given in English units because the code uses English units.

All IBM machine testing was performed on an AMDAHL 470V/8 machine using the IBM OS/VS2 (MVS) operating system and FORTRAN IV G1 Release 2.0 compiler. The AMDAHL machine uses the same data structure as the large mainframe IBM 370 series machines.

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PART 1
NOMENCLATURE

The following table of nomenclature applies to the report in general. Local definitions of variables that apply only to given sections of text are defined as they are encountered. English units are given for model parameters.

Units

Btu	British Thermal Units
°C	degrees centigrade
cp	centipoise
°F	degrees Fahrenheit
ft	feet
J	Joules
°K	degrees Kelvin
kg	kilogram
lbf	pound force, also lb
lbm	pound mass
m	meters or mass unit
md	millidarcy
psi	pounds per square inch
psia	pounds per square inch absolute
N	Newtons

W Watts

Upper Case Roman Letters

A an area--the portion of area is defined in the text (L^2)

ATES Aquifer Thermal Energy Storage

C solute concentration, mass fraction

[C] coefficient matrix--general

C_p heat capacity at constant pressure, Btu/(lbm °F) ($L^2t^{-2}T^{-1}$)

C_v heat capacity at constant volume ($L^2t^{-2}T^{-1}$)

D Hydrodynamic dispersion, ft²/day (L^2t^{-1})

D_m molecular diffusion, ft²/day (L^2t^{-1})

E "total" dispersivity--generalized (L^2t^{-1})

E_C "total" solute dispersivity, ft²/day (L^2t^{-1})

E_H "total" thermal dispersivity, Btu/(ft-day °F) ($mLt^{-3}T^{-1}$)

DOE U.S. Department of Energy

DWDM deep well disposal model

H enthalpy, Btu/lbm (L^2t^{-2})

J conversion from pressure to equivalent energy, 778.161 ft-lbf/Btu

K hydraulic conductivity, ft/day (Lt^{-1}) or thermal conductivity in general ($mLt^{-3}T^{-1}$)

K_H heat transfer coefficient through wellbore casing, Btu/(ft²-day °F) ($mL^2t^{-3}T^{-1}$)

K_m thermal conductivity of matrix, Btu/(ft-day °F) ($mLt^{-3}T^{-1}$)

L generalized length

LBL Lawrence Berkeley Laboratory

M mobility, ft³/(psi day) ($m^{-1}L^4t$)

NTIS National Technical Information Service

Nu	Nusselt number
P	thermodynamic related pressure ($\text{mL}^{-1}\text{t}^{-2}$)
$P_d(t_d)$	dimensionless pressure data from Van Everdingen and Hurst (1949). [PTD]
Pr	Prandlt number
Q	well volumetric flow rate (L^3t^{-1})
Q^*	quantity of substance--general
$\dot{Q}$	quantity of energy, Btu (mL^2t^{-2})
Q_w	well mass flow rate, lbm/day (mt^{-1})
{r}	designates residual column vector--general
Re	Reynolds number
S	generalized storage term--defined in text
T	temperature
T_E	total dispersivity transmission coefficient solute
T_H	total dispersivity transmission coefficient energy
T_w	transmission coefficient for pressure
U	internal energy, Btu/lbm (L^2t^{-2})
V	specific volume (L^3m^{-1}) in thermodynamic equations otherwise a volume (L^3), or when used with a directional subscript, i,j,k, refers to a velocity
W	water influx, ft^3 (L^3)
WSU	Washington State University
WI	well index (ft^2/day) (L^2t^{-1})

Lower Case Roman Letters

a_1	$= \partial \rho / \partial p \mid_{p=p_0}$
a_2	$= \partial \rho / \partial p \mid_{T=T_0}$
a_3	$= \partial \rho / \partial C \mid_{C=0}$
b	= reservoir thickness, ft (L)
c_R	= compressibility of rock, 1/psi ($m^{-1}Lt^2$)
c_T	= thermal expansion factor of water, 1/°F (T^{-1})
c_t	= total compressibility of matrix (definition varies in the text) ($m^{-1}Lt^2$)
c_w	= compressibility of water, 1/psi ($m^{-1}Lt^2$)
d	= a characteristic distance, or a characteristic grain diameter (L)
e_w	= water influx rate, ft ³ /day (L^3t^{-1})
$f(.)$	= function defined by text
fr	= pipe friction factor
g	= acceleration of gravity, 32.2 ft/sec ² (Lt^{-2})
g_c	= conversion factor (32.2 (ft-lbm)/(sec ² lbf)), for SI units $g_c =$ 1.0 (kg m)/(N(s) ²)
h	= convection heat transfer coefficient or elevation or hydraulic head, ft (L)
k	= permeability, millidarcy (L^2)
l	= length increment in flow direction
m	= mass, general
$o(.)$	= order of (.)
p	= pressure--usually in lbf/in ² ($mL^{-1}t^{-2}$)
q	= specific discharge or general darcy velocity, ft/day (Lt^{-1})
$\dot{q}$	= energy flow rate, general, Btu/day (mL^2t^{-3})
q_c	= colute flow rate lbm/day (mt^{-1})

q_H = conduction source term, Btu/(ft³ day) or heat loss rate, Btu/day
 q_L = conduction source term, Btu (mL²t⁻²)
 q_r = pore velocity, ft/day (Lt⁻¹)
 q_w = fluid source term, lbm/(ft³ day) or mass flow rate, lbm/day
 r = radius in general, ft (L)
 r_i = inner radius of casing, ft (L)
 r_o = outer radius of casing, ft (L)
 rb = radius measured to a grid block boundary, ft (L)
 rc = radius measured to a grid block center, ft (L)
 r_e = external grid block boundary radius or effective radius of reservoir, ft (L)
 r_n = radius measured to last grid block center, ft
 r_w = well radius, ft (L)
 t = time, days (t)
 t_d = dimensionless time
 u = general Darcy velocity or Darcy velocity x-direction, ft/day (Lt⁻¹)
 or dimensionless temperature
 $\tilde{u}$ = magnitude of Darcy velocity (Lt⁻¹)
 v = Darcy velocity y-direction (Lt⁻¹)
 v_i = an i-component of velocity - general term (Lt⁻¹)
 w = Darcy velocity z-direction (Lt⁻¹)
 x = direction related to x axis
 y = direction related to y axis, x-y coordinates make up the areal plane
 z = direction related to z axis or elevation

Greek Letters

α	weight function for first-order differencing upwind or central differencing (dimensionless) or thermal diffusivity, ft ² /day (L ² t ⁻¹)
α_l	Longitudinal dispersion coefficient, ft (L)
α_t	transverse dispersion coefficient, ft (L)
$\delta(.)$	change due to a time step
$\Delta(.)$	differential operator d(.)
η	general function defined in text
θ	angle measured about areal plane
ψ	angle measured from areal plane towards z-axis
μ	viscosity, cp (mL ⁻¹ t ⁻¹)
v_i	aquifer influence function coefficient $i = 1$ for pot aquifer; $i = 2$ for steady state aquifer
ξ	general function defined in text
ρ	density, in general or for water, lbm/ft ³ , (mL ⁻³)
ϕ	porosity

Functions

$\Gamma(x)$	$= \int_0^{\infty} t^{x-1} e^{-t} dt$, gamma function
$\text{erf}(x)$	$= 2/\sqrt{\pi} \int_0^x e^{-t^2} dt$, error function
$\text{erfc}(x)$	$= 1 - \text{erf}(x)$ complimentary error function
$\exp(x)$	$= e^x$ exponent
$\ln(x)$	$=$ natural log of x

Subscripts

bh	bottom-hole
C	concentration
d	dimensionless parameter

f	measured at saturation
g	grid point value
G	a "guessed" value or estimated value
H	refers to a heat transfer parameter of well casing, or heat transfer parameter in general
i	injected
i,j,k	subscripts referring to i-position, j-position and k-position in finite difference block arrangement
L	loss term, heat loss
m	medium, rock and water
o, o	base or initial value
ob	overburden value
p	pore value
r	reference or reservoir value
R	rock value
t	total value
ub	underburden value
w	water value
wb	wellbore
x	refers to x-direction
y	refers to y-direction
z	refers to z-direction
∞	far away, infinity or initial value

Superscripts

n	time level
---	------------

PART 2

TECHNICAL INFORMATION ON INTERCOMP CODE

INTRODUCTION

The INTERCOMP code is a completely self-contained package designed to solve pressure, energy, and single solute mass transport equations coupled with viscosity and density for laminar flow in porous media. The code allows a choice of one-, two-, or three-dimensional cartesian or two-dimensional radial coordinates and a variation in differencing techniques and boundary conditions. In addition, provisions are made for various printer output options, program restart, wellbore heat and pressure loss calculations, where the latter are important in deep well disposal problems.

This section consists of a summary of technical information about the simulator where listings of basic equations, assumptions, and outlines of the solution procedure are provided. References are made to original sources so that a user can further explore some of the assumptions involved. Rigorous mathematical derivation of the solution and all possible combinations are avoided to keep the explanation terse; hence, equations designated as forms may contain undefined coefficients as a result of grouping a series of variables. Emphasis is given to sections that are unclear in the original document (INTERCOMP, 1976).

A variable designated by $\bar{X}$ and $\overline{\overline{X}}$ are representations of first-order (vector) and second-order tensors, respectively. A statement $(d(Lt^{-1}))$ refers to a dimensional statement. Most of the generalized equations are given in standard vector notation, however, a few are written in standard indices or summation notation. The ∇ refers to an equation in vector notation, whereas Δ refers to an equation in finite-difference notation and Δ_x refers to differencing in the x-direction in particular. Variables given in capital letters enclosed in square brackets refer directly to input or computer code variables; for example, [CPW] is the fluid heat capacity, $(C_p)_w$ at constant pressure as found in the simulator. Since the simulator is written in English units, references to variables are given in English units rather than SI units (Le Systeme International d'Units). Quantities enclosed such as $(\rho C_p)_w$ (heat capacity per unit volume) refer to a quantity with respect to water. If a quantity such as ρ is given alone, it refers to water; however, if it is ρ_R , it refers to the rock material. Other similar subscript referrals are given in the section on nomenclature.

RESERVOIR MODEL

The INTERCOMP DWDM was designed to simulate the injection of waste in a deep isolated aquifer (reservoir). The model consists of two major parts: (a) a three-dimensional finite difference reservoir model and its associated boundary conditions, and (b) a wellbore model. The wellbore model relates surface conditions to downhole conditions or vice versa.

The basic capabilities of the reservoir simulator permit permit treatment of:

1. One-, two-, or three-dimensional transient laminar flow in a reservoir (aquifer), where permeability is treated as a first-order tensor;

2. Fluid density (ρ) as a function of pressure (p), temperature (T), and concentration (C);
3. Miscibility of injected fluids with reservoir fluids;
4. Aquifer properties such as porosity (ϕ), permeability ($\bar{k}$), thickness (b), and elevation (z) which vary with position and can be specified for each grid block (heterogeneity);
5. Hydrodynamic dispersion ($\bar{D}$) as a direct proportion of fluid velocity (u or q), and molecular diffusion phenomena ($\bar{D}_m$ or $\bar{K}_m$) which is additive to hydrodynamic dispersion. Hydrodynamic dispersion is accounted for by assuming an isotropic media based on a two-dimensional model described by Bear, 1961; and
6. The energy balance equation which is described as enthalpy (H) in - enthalpy out = change in internal energy for unsteady heat energy transport in the reservoir. Total internal energy change is the sum of internal energy in fluid at a given pressure and temperature and internal energy in rock at a given temperature.

RESERVOIR EQUATIONS

The momentum equation is

$$\bar{u} = \frac{-\bar{k}}{\mu} (\nabla p - \frac{\rho g}{g_c} \nabla z) \quad (2-1)$$

where u = darcy velocity (ft/day), μ = viscosity (cp), p = pressure (lbf/in²), ρ = density (lbm/ft³), g = acceleration of gravity, and z = vertical dimension (ft), increasing downward. This equation is also called Darcy's equation of motion (Darcy, 1856; Davis and DeWeist, 1966, p. 156), and can be derived from the generalized momentum equation by using the assumption that inertial forces are negligible in comparison to viscous forces which characterizes fluid flows having a low Reynolds number ($R_e = (\rho u d)/\mu$) in which d is grain diameter. The permeability ($\bar{k}$) in its general form is shown to be a second-order tensor (Bear, 1972, p. 109); however, the nine components are reduced to three by aligning the base coordinates to the principal direc-

thermal or thermodynamic equilibrium is also implied in equation (2-3) because of the lumping of the accumulation terms containing both internal energy in the fluid ($U(p,T)$) and in the solid ($(\rho C_p)_R T$). This assumption is valid for laminar fluid flow in porous media because the period of transient heat flow between the fluid and solid matrix consisting of small grains is short in comparison to heat transfer in the reservoir (Bear, 1972, p. 646). Additional details about the tensor quantity $\bar{\bar{E}}_H$ and the calculation of enthalpy and internal energy will be discussed later.

The third equation, which accounts for single solute mass balance, is written as:

$$\begin{array}{ccc}
 -\nabla \cdot (\rho \bar{u} C) & + & \nabla \cdot \rho \bar{\bar{E}}_C \cdot \nabla C & - & q_w C \\
 \text{(Net Concentration} & & \text{(Net Concentration} & & \text{(Net Concentration} \\
 \text{Convected)} & & \text{by Total Dispersion)} & & \text{by Source } q_w) \\
 & & & & \\
 & = & \frac{\partial}{\partial t} (\phi \rho C) & & (2-4) \\
 & & \text{(Accumulation)} & &
 \end{array}$$

This equation is similar in form to the one derived by B.S.L., p. 557, without the source term $q_w C$ ($d(\text{mL}^{-3}\text{t}^{-1})$). The C is defined as the mass fraction ρ_C/ρ . Equation (2-4) differs from B.S.L. in its definition of $\bar{\bar{E}}_C$ and its lack of a term that represents the "creation" of the substance due to a chemical conversion. Since the region occupied by the tracer is limited to the void space, the accumulation term is $\phi \rho C$ rather than ρC .

Equation (2-1) is combined with equations (2-2), (2-3), and (2-4) to give:

$$\nabla \cdot \left(\rho \frac{\bar{k}}{\mu} \left(\nabla p - \frac{\rho g}{g_c} \nabla z \right) \right) - q_w = \frac{\partial}{\partial t} (\phi \rho) \quad (2-5)$$

$$\begin{aligned} \nabla \cdot (\rho_H \frac{\bar{k}}{\mu} (\nabla p - \frac{\rho g}{g_c} \nabla z)) + \nabla \cdot \bar{\bar{E}}_H \cdot \nabla T - q_H - q_w^H \\ = \frac{\partial}{\partial t} (\phi \rho U + (1 - \phi) (\rho C_p)_R T) \end{aligned} \quad (2-6)$$

and

$$\begin{aligned} \nabla \cdot (\rho_C \frac{\bar{k}}{\mu} (\nabla p - \frac{\rho g}{g_c} \nabla z)) + \nabla \cdot \rho_C \bar{\bar{E}}_C \cdot \nabla C - q_w^C \\ = \frac{\partial}{\partial t} (\phi \rho C). \end{aligned} \quad (2-7)$$

These are the governing equations used in the simulator, where equation (2-5) is always solved, with options to solve both equations (2-6) and (2-7) in that order, or combinations of equations (2-5) and (2-6), or (2-5) and (2-7) or (2-5) alone.

Equations (2-6) and (2-7) contain terms of similar form. Two terms in particular are $\bar{\bar{E}}_H$ and $\bar{\bar{E}}_C$. The model defines

$$\bar{\bar{E}}_H = \bar{\bar{\Phi}}_H + \bar{K}_m \quad d(mLt^{-3}T^{-1}) \quad (2-8)$$

and

$$\bar{\bar{E}}_C = \bar{\bar{\Phi}}_C + \bar{D}_m \quad d(L^2t^{-1}) \quad (2-9)$$

where $\bar{K}_m$ and $\bar{D}_m$ represent coefficients for molecular transport of energy (effective thermal conductivity of fluid and matrix) and molecular diffusion through the porous media. The term $\bar{K}_m$ is treated as a first-order tensor and is allowed directional variability, while $\bar{D}_m$ is treated as a constant in all directions. The general mechanical dispersion coefficient $\bar{\bar{\Phi}}$ is treated as a second-order tensor whose value is dependent upon a simple proportionality with the magnitude of the Darcy velocity (u). The summation of the mechanical dispersion and molecular diffusion coefficients accounts for the general total

dispersion coefficient $\bar{E}$ (Bear, 1972, p. 650). Physically, this term accounts for the spreading of a temperature or solute front in the porous media. Forms represented by equations (2-8) and (2-9) are a simplification of the most general case where

$$\bar{E} = \bar{D} + \bar{D}_m$$

as described by Bear, 1972, p. 606.

For an isotropic medium, Scheidegger (1961), has shown that there can be no more than two independent mechanical dispersion factors. These are best described as the longitudinal and transverse mechanical dispersion coefficients $(d(L)) \alpha_l$ and α_t , respectively. Bear (1961) analyzed the mechanical spreading phenomena using a form

$$\bar{D}_{kl} = a_{ijkl} \frac{v_i v_j}{u} = \bar{D}_C u$$

where a_{ijkl} is a fourth-order tensor describing the medium dispersivity, u is the magnitude of Darcy velocity, and v_i and v_j are Darcy velocities in the i th and j th directions. The components of $\bar{D}_C$ are given in Bear's (1961) paper for isotropic media in two dimensions, and when expanded to three dimensions the results are

$$D_{11} = D_{xx} = \alpha_l \cos^2 \psi \cos^2 \theta + \alpha_t (\sin^2 \theta \cos^2 \psi + \sin^2 \psi)$$

$$D_{12} = D_{xy} = (\alpha_l - \alpha_t) \sin \theta \cos \theta \cos^2 \psi$$

$$D_{13} = D_{xz} = (\alpha_l - \alpha_t) \sin \psi \cos \psi \cos \theta$$

$$D_{yx} = D_{xy}$$

$$D_{22} = D_{yy} = \alpha_l \cos^2 \psi \sin^2 \theta + \alpha_t (\cos^2 \theta \cos^2 \psi + \sin^2 \psi)$$

20

$$D_{23} = D_{yz} = (\alpha_l - \alpha_t) \sin \psi \cos \psi \sin \theta$$

$$D_{zx} = D_{xz}$$

$$D_{33} = D_{zz} = \alpha_l \sin^2 \psi + \alpha_t \cos^2 \psi$$

$$D_{zy} = D_{yz} \quad (2-10)$$

where θ is the angle of the fluid flow in the x-y plane and ψ is the flow angle measured from the x-y plane in the z-direction. The terms $\bar{D}_H$ and $\bar{D}_C$ in equations (2-8) and (2-9) are related by

$$\bar{D}_H = \bar{D}_C (\rho C_p)_w$$

where $(\rho C_p)_w$ is the heat capacity of water per unit volume. The terms listed in equation (2-10) are used in equation (2-7) in the following manner:

$$\begin{aligned} \nabla \cdot \bar{E}_C \cdot \nabla C &= \frac{\partial}{\partial x} (E_{xx} \frac{\partial C}{\partial x}) + \frac{\partial}{\partial x} (E_{xy} \frac{\partial C}{\partial y}) + \frac{\partial}{\partial x} (E_{xz} \frac{\partial C}{\partial z}) \\ &+ \frac{\partial}{\partial y} (E_{yx} \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} (E_{yy} \frac{\partial C}{\partial y}) + \frac{\partial}{\partial y} (E_{yz} \frac{\partial C}{\partial z}) \\ &+ \frac{\partial}{\partial z} (E_{zx} \frac{\partial C}{\partial x}) + \frac{\partial}{\partial z} (E_{zy} \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z} (E_{zz} \frac{\partial C}{\partial z}) \end{aligned}$$

where

$$E_{xx} = D_{xx} \tilde{u} + D_m$$

$$E_{xy} = D_{xy} \tilde{u}$$

$$E_{yy} = D_{yy} \tilde{u} + D_m$$

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and likewise for equation (2-6) except that the thermal molecular transport term changes with direction.

Equations (2-5), (2-6), and (2-7) are interconnected by density, viscosity, and enthalpy models. Density is a function of temperature, pressure, and concentration; viscosity is a function of temperature and concentration; and enthalpy is a function of pressure and temperature in the model. In theory, the density and viscosity models are known as the equations of state.

DENSITY MODEL

The density model is best described as:

$$\begin{aligned} \rho(p, T, C) = & \rho_0(p_0, T_0, 0) + \left(\frac{\partial \rho}{\partial p} \right) \bigg|_{p=p_0} (p - p_0) + \dots \\ & + \left(\frac{\partial \rho}{\partial T} \right) \bigg|_{T=T_0} (T - T_0) + \dots + \left(\frac{\partial \rho}{\partial C} \right) \bigg|_{C=0} (C) + \dots \end{aligned} \quad (2-11)$$

where ρ is given in pound-mass (lbm). This description comes from a three-dimensional Taylor series expansion that deals with natural reservoir fluid properties at base pressure p_0 , base temperature T_0 , and zero concentration of injection fluid. In the model, equation (2-11) is written as:

$$\rho(p, T, C) = \rho_0 + a_1(p - p_0) + a_2(T - T_0) + a_3(C) \quad (2-12)$$

where constants

$$a_1 = \left(\frac{\partial \rho}{\partial p} \right) \bigg|_{p=p_0}$$

$$a_2 = \left. \frac{\partial \rho}{\partial T} \right|_{T=T_0}$$

and

$$a_3 = \left. \frac{\partial \rho}{\partial C} \right|_{C=0}.$$

These constants are determined from the isothermal water compressibility

$$c_w = \frac{1}{\rho_0} \left(\frac{\partial \rho}{\partial p} \right)_T \quad [CW]$$

and the water thermal expansion factor

$$c_T = - \frac{1}{\rho_0} \left(\frac{\partial \rho}{\partial T} \right)_p \quad [-CTW]$$

where $)_p$ and $)_T$ signify constant pressure and temperature, respectively.

Therefore,

$$a_1 = \left. \frac{\partial \rho}{\partial p} \right|_{T_0, C_0} = \rho_0 c_w$$

$$a_2 = - \left. \frac{\partial \rho}{\partial T} \right|_{p_0, C_0} = \rho_0 c_T$$

and

$$a_3 = \left. \frac{\partial \rho}{\partial C} \right|_{C=0} = \rho(p_r, T_r, 1) - \rho(p_r, T_r, 0)$$

where $\rho(p_r, T_r, 1)$ and $\rho(p_r, T_r, 0)$ are the injection fluid density [BWRI] and reservoir fluid density [BWRN] at reference pressure p_r [PBWR] and reference temperature T_r [TBWR], respectively. The simulator computes the base density ρ_0 by considering the initial reservoir pressure p_0 [PINIT] and base temperature T_0 [T0] by

$$\rho_0 = \frac{\rho_r}{1 + c_w(p_r - p_0) + c_T(T_r - T_0)}.$$

VISCOSITY MODEL

The viscosity model is dependent upon the types of data that are available. In summary, the changes in viscosity are a function of both temperature and concentration. Since viscosity is usually a weak function of pressure, pressure effects are disregarded.

The formulation of the viscosity model is

$$\mu(T, C) = \mu(T_r, C) \exp \left[B(C) \left(\frac{1}{T} - \frac{1}{T_r} \right) \right] \quad (2-13)$$

where

$\mu(T_r, C)$ = fluid viscosity at reference temperature (T_r)
given as an input data [NCV>0], or

$$\mu(T_r, C) = \mu_i(T_r)^C \mu_r(T_r)^{(1-C)} \quad (2-14)$$

[VISIR] [VISRR]

when only pure component data are available [NCV=0]. The compositional factor B is determined as

$$B(C) = CB_i + (1 - C)B_r \quad (2-15)$$

where subscripts i and r refer to injection and reservoir, respectively, and B_i and B_r are "best constants" calculated from linear interpolation of temperature data in the injection and reservoir fluids, respectively.

The model operates by first solving for B_i and B_r and retaining these values as constants. Further viscosity calculations require only equation (2-14) or the data table on viscosity vs. concentration at reference temperature and equations (2-15) and (2-13).

The level of accuracy of the model depends upon the types of viscosity data that are available. Data entry options are as follows:

(A) Input Quantity

$\mu(T_r, C)$ - viscosity of fluid mixture as a function of composition at reference temperature ([NCV]>0).

$\mu_i(T)$ - viscosity of injection fluid as a function of temperature ([NTVI]>0).

$\mu_r(T)$ - viscosity of resident (reservoir) fluid as a function of temperature ([NTVR]>0).

Model calculates:

B_i and B_r as a least square fit of $\mu_i(T)$ and $\mu_r(T)$. The $\mu(T_r, C)$ is interpolated from input table, and $\mu(T, C)$ is determined by equations (2-15) and (2-13).

(B) Input Quantity

$\mu_i(T)$, $\mu_r(T)$ - viscosities of injected and resident fluids as functions of temperature ($[NTVI]>0$, $[NTVR]>0$, and $[NCV=0]$).

Model calculates:

B_i and B_r from least squares fit of μ_i and μ_r . The $\mu(T_r, C)$ is determined by equation (2-14), and $\mu(T, C)$ is calculated by equations (2-15) and (2-13).

(C) Input Quantity

$\mu_i(T_r)$, $\mu_r(T_r)$ - viscosities of injected and reservoir fluids at a single temperature (T_r).

Model calculates:

B_i and B_r are calculated from internal data from generalized viscosity from Lewis and Squire, 1934 and Perry, 1963. The $\mu(T_r, C)$ is determined from equation (2-14) and $\mu(T, C)$ from equations (2-15) and (2-13).

Note: In all the above calculations, T_r is assumed to be the same for both resident and injection fluid; however, the model has provisions to handle different reference temperatures for injection fluid $[TIR]$ and reservoir fluid $[TRR]$. Best results are obtained when $[TRR] = [TIR]$.

Based on the above discussion, one must specify reference viscosity and additional viscosity data in order to specify the independence of viscosity from temperature and/or concentration because Lewis and Squire's chart is used when reference viscosities are the only data specified.

According to INTERCOMP, the expected accuracy of the viscosity model, at most, results in a 5 to 15% difference between the calculated and measured viscosities between 0° C (32° F) and 100° C (212° F) for pure water, with probable larger deviations when dealing with fluids other than pure water. Better accuracy is obtained when more data are available. The larger deviations are caused by poor correlation of the Lewis-Squire data with water containing higher levels of contaminants.

ENTHALPY MODEL

Energy balance is written in terms of enthalpy in - enthalpy out = change in internal energy. This section describes the method used by the simulator to account for enthalpy and its related components (p,T). The enthalpy of water [EH] is computed as

$$H = U_0 + C_p (T - T_0) + \frac{J}{\rho} (p) \quad (2-16)$$

where U_0 is a base internal energy [UW0], C_p is a constant water heat capacity at constant pressure [CPW], and J is the pressure work conversion [CNV] = 144 in²/ft²/778.2 ft-lbf/Btu). The reference enthalpy U_0 is determined by using data presented in Tables 2-1 and 2-2. The model calculations are as follows:

$$U_0 = f_1(T_0) + f_2(T_0, p_0) - J \frac{p_0}{\rho_0} \quad (2-17)$$

where $f_1(T_0)$ is the best value obtained by linear interpolation of the saturated enthalpy in Table 2-1, and $f_2(T_0, p_0)$ is the deviation from saturation ($H = H_f$) obtained from two-dimensional linear interpolation of Table 2-2. Base values T_0 , p_0 , and ρ_0 are the same as those defined in the density model. Tables 2-1 and 2-2 are similar to more complete data tables found in Keenan and Keyes, (1964, pp. 27-39 and p. 89, respectively). The last term in equation (2-17) subtracts the effects of base pressure p_0 so that H at a new pressure, p is calculated by adding only the effects of the new pressure in equation (2-16).

Bottom-hole temperatures in the production wells are computed from the grid block enthalpy (H) and pressure (p) values by an iterative technique.

The basic method starts by assigning a value of bottom-hole temperature (T_G) and calculating the enthalpy from

$$T_G^{l+1} = [T_G + \left(\frac{H - H_L}{H_H - H_L} \right) (T_H - T_L)]^l$$

and

$$H_G = f_1(T_G) + f_2(T_G, p)$$

where subscripts H and L represent the high and low values from the previous iteration step. The low or high enthalpy and temperatures are updated with proper "guessed" values (H_G and T_G) until the following is satisfied:

$$\frac{|H_G - H|}{H} \leq \text{tol} \quad [\text{EPS}].$$

where H_G refers to the present estimate of enthalpy, and tol refers to a prescribed tolerance.

Table 2-1. Enthalpy of Saturated Water

Temperature [TSW] (°F)	Enthalpy [EHW] (Btu/lbm)
32.0	0.0
60.0	28.06
90.0	57.99
120.0	87.92
150.0	117.89
180.0	147.92
212.0	180.1
240.0	208.4
281.0	250.1
307.6	277.4
327.8	298.1
358.4	330.5
381.8	355.4
400.9	376.0
417.3	393.9
444.6	424.0
467.0	449.4
486.2	471.6
503.1	491.5
518.2	509.7
531.9	526.6
544.6	542.4
567.2	571.7
587.1	598.6
604.9	623.9
621.0	648.0
635.8	671.7
668.1	730.7
705.31	910.3

Equation (2-16) is based on an equivalent thermodynamic identity given in B.S.L. (p. 315) where

$$dU = \left(\frac{\partial U}{\partial V}\right)_T dV + \left(\frac{\partial U}{\partial T}\right)_V dT = [-p + T\left(\frac{\partial p}{\partial T}\right)_V] dV + C_V dT \quad (2-18)$$

Table 2-2. Compressed Water Enthalpy

$$(H - H_f)$$

Pressure (psia) [PLW]	100	200	300	400	500	600	660	700 Temperature (°F) [TLW]
200	.54	.41	.23	0.	0.	0.	0.	0.
600	1.67	1.31	.97	.39	0.	0.	0.	0.
1000	2.70	2.21	1.75	.84	-.14	0.	0.	0.
1500	3.99	3.36	2.70	1.44	-.29	0.	0.	0.
2000	5.31	4.51	3.64	2.03	-.38	-2.5	0.	0.
2500	6.58	5.63	4.55	2.66	-.41	-4.6	-3.1	0.
3000	7.88	6.76	5.49	3.33	-.41	-6.9	-11.8	0.
3500	9.17	7.90	6.44	4.01	-3.40	-8.60	-17.8	-42.8
4000	10.5	9.03	7.41	4.70	-.16	-10.0	-22.5	-59.5
4500	11.8	10.15	8.40	5.40	.02	-11.1	-26.4	-69.8
5000	13.1	11.3	9.36	6.08	.25	-12.0	-29.5	-76.9
5500	14.4	12.5	10.36	6.78	.52	-13.0	-31.8	-82.0

where U is internal energy, V is specific volume, and C_v is heat capacity at constant volume. Equation (2-18) is useful in simplifying the accumulation term of an energy equation written in terms of internal energy. The equivalent term for an equation written for changes in enthalpy is (Abbott and Van Ness, p. 78):

$$dH = \left(\frac{\partial H}{\partial T}\right)_P dT + [V - T \left(\frac{\partial V}{\partial T}\right)_P] dp$$

which can be approximated as

$$dH = C_p dT + [V]dp \quad (2-19)$$

where the expansion coefficient is considered negligible. Here, the variable V is specific volume, and the product (PV) has dimensions of energy per unit mass. Equation (2-16) can be derived from equation (2-19).

The model allows for only one value of C_p for both the injection and reservoir fluids. This assumption is best when the solute injected is water-based, and the contaminant in solution is dilute.

The enthalpy of the rock component is given by

$$H_R = U_R + (PV)_R \quad (2-20)$$

The change in H_R is

$$dH_R = dU_R + d(PV)_R$$

where for a solid, $d(PV)_R$ is approximately zero and is treated as such in the model, resulting in

$$H_R = U_R = (C_p)_R (T - T_0)$$

where T_0 is the base temperature $[T_0]$ for the fluid enthalpy model selected by the user.

Energy in place is computed by assuming a variable pore volume

$$V_p = \phi_0 V_t$$

$$V_w = V_p (1 + c_R (p - p_0))$$

where V_t = total volume, ϕ_o = user-defined porosity, V_p = pore volume at initial pressure [PINIT], and c_R is the rock compressibility. The energy in place is

$$\dot{Q}' = \rho V_w (U_0 + C_p (T - T_0)) + (V_t - V_p) (\rho C_p)_R (T - T_0) . \quad (2-21)$$

Note that the energy is computed by assuming a variable pore volume, V_w to compute the fraction of energy in the fluid; however, a constant volume of rock is used to compute energy in the rock mass. In relation to equation (2-21) the mass of water in place is

$$Q' = \rho V_w \quad (2-22)$$

and the solute mass in place is

$$Q'_C = \rho V_w C . \quad (2-23)$$

Quantities derived from equations (2-21), (2-22), and (2-23) are evaluated on a block by block basis, and the summation of all quantities in each block gives the total for the reservoir domain.

FINITE DIFFERENCE SOLUTION METHOD

This section is a summary of the method used to reduce the governing equations to a form that can be solved. A number of equations are designated as forms that contain undefined coefficients, which are the result of combining groups of variables.

Equations (2-5), (2-6), and (2-7) are written in finite difference form as follows:

$$\Delta[T_w(\Delta p)] - q_w^* = \frac{V}{\Delta t} \delta(\phi\rho) \quad (2-24)$$

$$\begin{aligned} \Delta[HT_w(\Delta p)] + \Delta[T_H \Delta T] - q_H^* - q_w^* \\ = \frac{V}{\Delta t} \delta(\phi\rho U + [(1 - \phi)(\rho C_p)_R T]) \end{aligned} \quad (2-25)$$

and

$$\Delta[CT_w(\Delta p)] + \Delta[T_E \Delta C] - Cq_w^* = \frac{V}{\Delta t} \delta(\phi\rho C) \quad (2-26)$$

where

$$V = \Delta x_i \Delta y_j \Delta z_k \quad \text{or} \quad 2\pi(r b_i^2 - r b_{i-1}^2) \Delta z_k$$

$$\Delta(\cdot) = (\cdot)_i - (\cdot)_{i-1}$$

$$\Delta \bar{p} = (\Delta p - \frac{\rho g}{g_c} \Delta z)$$

$$\Delta T_w \Delta \bar{p} = \Delta_x (T_w \Delta_x \bar{p}) + \Delta_y (T_w \Delta_y \bar{p}) + \Delta_z (T_w \Delta_z \bar{p})$$

$$\Delta T_H \Delta T = \Delta_x (T_H \Delta_x T) + \Delta_y (T_H \Delta_y T) + \Delta_z (T_H \Delta_z T)$$

$$\text{with } \Delta_x (T_H \Delta_x T) = \Delta_x T_{H_{xx}} \Delta_x T + \Delta_x T_{H_{xy}} \Delta_y T + \Delta_x T_{H_{xz}} \Delta_z T$$

and a similar expansion for $\Delta T_E \Delta C$. The actual form used in the last expansion depends upon the data entered; hence, a more detailed explanation will come later in this discussion. The right-hand side of equation (2-24) is expanded as follows:

$$\delta(\phi\rho) = (\phi\rho)^{n+1} - (\phi\rho)^n \quad (2-27)$$

in which the superscript, n , represents a time level. Similar expansions are applied to equations (2-25) and (2-26). The transmission coefficients (transmissibilities), without reference to direction, are defined as

$$\begin{aligned} T_W &= \frac{kA\rho}{\mu \ell} & [TXW, TYW, TZW] \\ T_H &= \frac{E_H A}{\ell} & [TXH, TYH, TZH] \\ T_E &= \frac{E_C A\rho}{\ell} & [TXG, TYG, TZG] \end{aligned} \quad (2-28)$$

where A represents the area on a grid block face, normal to the flux direction, and ℓ is a length over which the gradient ($\Delta\rho$, ΔC , or ΔT) is measured, in the direction of the flux. From the above discussion, equations (2-24), (2-25), and (2-26) are derived from equations (2-5), (2-6), and (2-7), which are multiplied through by a finite difference grid volume (Δx , Δy , and Δz). The dimensions of equations (2-24), (2-25), and (2-26) are now lbm/day, $(d(mt^{-1}))$, Btu/day $(d(mL^2t^{-3}))$ and lbm/day $(d(mt^{-1}))$, respectively.

Further expansions of transmission coefficients in equation (2-28) are written as

$$T_{W_{i-\frac{1}{2},j,k}} = \frac{2\Delta y_i \Delta z_k}{\left(\frac{\Delta x}{k_x}\right)_i + \left(\frac{\Delta x}{k_x}\right)_{i-1}} \left(\frac{\rho}{\mu}\right)_{i-\frac{1}{2},j,k} \quad [TXW] \quad (2-28-a)$$

$$T_{H_{i,j-\frac{1}{2},k}} = \frac{2\Delta x_i \Delta z_k}{\left(\frac{\Delta y}{E_H}\right)_j + \left(\frac{\Delta y}{E_H}\right)_{j-1}} \quad [TYH] \quad (2-28-b)$$

and

$$T_{E_{i,j,k-\frac{1}{2}}} = \frac{2\Delta x_i \Delta y_j}{\left(\frac{\Delta z}{E_C}\right)_k + \left(\frac{\Delta z}{E_C}\right)_{k-1}} \rho_{i,j,k-\frac{1}{2}} \quad [TZG] \quad (2-28-c)$$

where the subscript locations are shown in Figure (2-1). For radial geometry, the above forms become

$$T_{w_{i-\frac{1}{2},k}} = \frac{2\pi (rb)_i k_{i-\frac{1}{2}} \Delta z_k}{[(rc)_i - (rc)_{i-1}] \left(\frac{\rho}{\mu}\right)_{i-\frac{1}{2},k}} \quad [\text{TXW}] \quad (2-28-d)$$

and

$$T_{w_{i,k-\frac{1}{2}}} = \frac{2\pi ((rb)_{i+1}^2 - (rb)_i^2) k_{i,k-\frac{1}{2}} \Delta z_k}{\Delta z_k + \Delta z_{k-1}} \left(\frac{\rho}{\mu}\right)_{i,k-\frac{1}{2}} \quad [\text{TZW}] \quad (2-28-e)$$

where rb_i = radius at grid block boundary, between two grid block centers rc_i and rc_{i-1} . The boundary radius rb_i is determined by using equation 13 in Settari and Aziz (1974), given as

$$rb_i = \frac{rc_i - rc_{i-1}}{\ln\left(\frac{rc_i}{rc_{i-1}}\right)}$$

This form is used because of desirable integral properties which give the best discretization accuracy when logarithmic mean radius is used.

One can show this by recalling the Laplacian in radial coordinates as

$$\Delta T_w^* \Delta h = \frac{1}{r} \frac{\partial}{\partial r} (2\pi K r b \frac{\partial h}{\partial r})$$

or

$$\frac{1}{r} \frac{\partial}{\partial r} (2\pi K b r \frac{\partial h}{\partial r}) \approx \frac{1}{rc_i (\Delta rc_i)} [q_{i-\frac{1}{2}}^* - q_{i+\frac{1}{2}}^*]$$

Figure 2-1. Generalized reservoir finite difference molecule

where

$$-q^* = 2\pi K r b \frac{\partial h}{\partial r} = 2\pi K b \frac{\partial h}{\partial (\ln r)}$$

and after discretizing

$$-q_{i-\frac{1}{2}}^* = 2\pi K_{i-\frac{1}{2}} b \frac{h_i - h_{i-1}}{\ln\left(\frac{rc_i}{rc_{i-1}}\right)}$$

where b is the thickness of the section, and K is given in $d(Lt^{-1})$ and h in $d(L)$.

The convective terms in equations (2-25) and (2-26) are weighted, depending upon the type of differencing option selected by the user. For example, the net convected concentration calculated at the old time level in the i th block is

$$C_{i-\frac{1}{2}} q_{w_{i-\frac{1}{2}}} - C_{i+\frac{1}{2}} q_{w_{i+\frac{1}{2}}} = \Delta_x [C T_w \Delta_x \bar{p}] \quad (2-28-f)$$

where C and q_w are evaluated at the left and right boundaries of a grid block (Figure 2-1-B). The grid block boundary concentration C is evaluated by

$$C_{i-\frac{1}{2}} = \alpha C_{i-1} + (1 - \alpha) C_i \quad (2-28-g)$$

where $\alpha = .5$ for central differencing, and $\alpha = 1$ for upwind differencing if flow is from left to right ($q_{w_{i-\frac{1}{2}}} \geq 0$) in Figure 2-1-B, and $\alpha = 0$ if flow is from right to left ($q_{w_{i-\frac{1}{2}}} < 0$). For the energy equation, C is replaced by H .

The net total dispersive flux calculated at the old time level in a grid block is

$$T_{E_{i-\frac{1}{2}}}(C_{i-1} - C_i) - T_{E_{i+\frac{1}{2}}}(C_i - C_{i+1}) = \Delta_x (T_E \Delta_x C) \quad (2-28-h)$$

where $T_{E_{i-\frac{1}{2}}}$ and $T_{E_{i+\frac{1}{2}}}$ are defined earlier as the harmonic average of the total dispersivity between two grid block centers where

$$T_{E_{i-\frac{1}{2}}} = [(\alpha_{\ell} \tilde{u})_{i-\frac{1}{2}} + D_m] \left(\frac{A\rho}{\ell} \right)_{i-\frac{1}{2}} \quad (2-28-i)$$

for one-dimensional flow in the x-direction. When the flow rate is zero, the means of transport become diffusion, defined by coefficient D_m . As a result of the above discussion, the "temporary" residual evaluated for a block without a source becomes

$$\begin{aligned} & C_{i-\frac{1}{2}} q_{w_{i-\frac{1}{2}}} - C_{i+\frac{1}{2}} q_{w_{i+\frac{1}{2}}} + T_{E_{i-\frac{1}{2}}}(C_{i-1} - C_i) \\ & - T_{E_{i+\frac{1}{2}}}(C_i - C_{i+1}) = RC_i \quad [RC] \end{aligned} \quad (2-28-j)$$

In a generalized three-dimensional problem with minimum outer iterations in the solving algorithm [MINITN] set as greater than one, the dispersive flux is calculated as

$$\begin{aligned} \Delta [T_E \Delta C] &= \Delta_x [T_{E_{xx}} \Delta_x C] + \Delta_x [T_{E_{xy}} \Delta_y C]^{\ell-1} \\ &+ \Delta_y [T_{E_{yx}} \Delta_x C]^{\ell-1} + \Delta_y [T_{E_{yy}} \Delta_y C] + \Delta_z [T_{E_{zz}} \Delta_z C] \end{aligned} \quad (2-28-k)$$

where $\ell-1$ indicates the use of the value from the previous iteration where

$$T_{E_{xx}} = [D_{xx} \tilde{u} + D_m] \frac{A\rho}{\ell}$$

$$T_{E_{yx}} = T_{E_{xy}} = [D_{xy} \tilde{u}] \frac{A\rho}{\ell}$$

$$T_{E_{YY}} = [D_{YY} \tilde{u} + D_m] \frac{A\rho}{l}$$

$$T_{E_{ZZ}} = [(D_{ZZ} + D_{XZ} + D_{YZ}) \tilde{u} + D_m] \frac{A\rho}{l}$$

where

$$\frac{A\rho}{l}$$

depends upon the direction in which ΔC is being evaluated. If the minimum number of iterations [MINITN] is set as one, the dispersive flux is estimated as

$$\Delta T_E \Delta C = \Delta_x [T_{E_{xx}} \Delta_x C] + \Delta_y [T_{E_{yy}} \Delta_y C] + \Delta_z [T_{E_{zz}} \Delta_z C] \quad (2-28-1)$$

where

$$T_{E_{xx}} = [(D_{xx} + D_{xy}) \tilde{u} + D_m] \frac{A\rho}{l}$$

$$T_{E_{yy}} = [(D_{yy} + D_{xy}) \tilde{u} + D_m] \frac{A\rho}{l}$$

$$T_{E_{zz}} = [(D_{zz} + D_{xz} + D_{yz}) \tilde{u} + D_m] \frac{A\rho}{l}$$

Similar forms are used in calculating the net dispersive energy flux with allowance for directional changes in molecular transport of energy ($\bar{K}_m$).

The simulator treats water as a slightly compressible fluid. A similar allowance is applied to the matrix; hence, in general the right hand sides of equations (2-24), (2-25), and (2-26) are expanded as follows:

$$\delta(ab) = (ab)^{n+1} - (ab)^n = a^{n+1}b^{n+1} - a^{n+1}b^n + a^{n+1}b^n + a^n b^n$$

or

$$\delta(ab) = a^{n+1}\delta b + b^n\delta a$$

Applying the above specifically to equation (2-24), the following is obtained:

$$\frac{V}{\Delta t} \delta(\phi\rho) = \frac{V}{\Delta t} (a_1\phi^n\delta p + a_2\phi^n\delta T + a_3\phi^n\delta C + \rho^{n+1}\phi_0c_R\delta p) \quad (2-29)$$

in which

$$a_1 = \left. \frac{\partial \rho}{\partial p} \right|_{T_0, C_0}$$

$$a_2 = \left. \frac{\partial \rho}{\partial T} \right|_{p_0, C_0}$$

$$a_3 = \left. \frac{\partial \rho}{\partial C} \right|_{p_0, T_0}$$

were defined earlier in the density model and ϕ_0 = user-defined base porosity. The last term in equation (2-29) represents the effect of compressibility of the rock matrix. The similar expansion for equation (2-25) is

$$\begin{aligned} \frac{V}{\Delta t} \delta(\phi\rho U + [(1 - \phi)(\rho C_p)_R]T) &= \frac{V}{\Delta t} (a_1\phi^n U^n \delta p + a_2\phi^n U^n \delta T + a_3\phi^n U^n \delta C \\ &+ \phi^{n+1}(\rho^{n+1} C_p)_w \delta T + \rho^{n+1} U^n \phi_0 c_R \delta p \\ &+ (\rho C_p)_R \delta T - \phi^{n+1}(\rho C_p)_R \delta T - T^n(\rho C_p)_R \phi_0 c_R \delta p) \end{aligned} \quad (2-30)$$

and for equation (2-26)

$$\begin{aligned} \frac{V}{\Delta t} \delta(\phi \rho C) = \frac{V}{\Delta t} (a_1 \phi^n C^n \delta p + a_2 \phi^n C^n \delta T + a_3 \phi^n C^n \delta C \\ + \rho^{n+1} C^n \phi_0 c_R \delta p + \rho^{n+1} \phi^{n+1} \delta C) \end{aligned} \quad (2-31)$$

The flowing source terms are written as

$$-q_w^* = (q_{w_i}^n + \frac{dq_{w_i}}{dp} \delta p) - (q_{w_o}^n + \frac{dq_{w_o}}{dp} \delta p) \quad (2-32)$$

where subscripts i and o refer to flow in and out, respectively. The source (or sink) are broken into two parts for greater solution accuracy and stability. The q_i^n and q_o^n are the explicit part, or flow rate at the old time level, and $(dq_i/dp)\delta p$ and $(dq_o/dp)\delta p$ are the additional flow rates due to change in pressure over a time step (implicit part).

After moving the right side to left, and left side to right in equations (2-24), (2-25) and (2-26), and regrouping variables, the following forms are obtained:

$$C_{11}\delta C + C_{12}\delta T + C_{13}\delta p = (\Delta CT_w \bar{\Delta p}) + R_1^* \quad (2-33)$$

$$C_{21}\delta C + C_{22}\delta T + C_{23}\delta p = (\Delta HT_w \bar{\Delta p}) + R_2^* \quad (2-34)$$

and

$$C_{31}\delta C + C_{32}\delta T + C_{33}\delta p = (\Delta T_w \bar{\Delta p}) + R_3^* \quad (2-35)$$

respectively. The "C" terms on the left side are coefficients associated with unknowns δC , δT , and δp , which are part of the accumulation terms, and

terms on the right sides are designated as residuals. One should note that at this stage, the residuals still contain implicit terms. After combining equations (2-33), (2-34), and (2-35), and using Gaussian elimination, the resultant equations have a form of

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ 0 & C'_{22} & C'_{23} \\ 0 & 0 & C''_{33} \end{bmatrix} \begin{Bmatrix} \delta C \\ \delta T \\ \delta p \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ C_{24} & 1 & 0 \\ C'_{34} & C_{35} & 1 \end{bmatrix} \begin{Bmatrix} \Delta [CT_w \Delta \bar{p}] \\ \Delta [HT_w \Delta \bar{p}] \\ \Delta [T_w \Delta \bar{p}] \end{Bmatrix} + \begin{Bmatrix} R_1^* \\ R_2'^* \\ R_3''^* \end{Bmatrix} \quad (2-36)$$

or

$$[C]\{x\} = [G]\{H\} + \{R^*\} \quad (2-36-a)$$

This form allows one to solve for δp , followed by δT and δC , respectively. For example, the pressure equation has the form

$$[C''_{33}]\{\delta p\} = C'_{34}\Delta T_w \Delta \bar{p} + C_{35}\Delta T_w H \Delta \bar{p} + \Delta T_w \Delta \bar{p} + R_3''^* \quad (2-37)$$

where each component on the right side contains implicit and explicit parts.

An example of an expansion on the right side is

$$(\Delta T_w \Delta \bar{p})^{n+1} = \Delta T_w \Delta \bar{p}^n + \Delta T_w \Delta (\delta p) - \Delta T_w \rho^n \frac{g}{g_c} \Delta z$$

where $p^{n+1} = p^n + \delta p$. The items with superscript, n , are known and are kept on the right side of equation (2-37). After separating implicit and explicit components, equation (2-37) has a form of

$$[C]\{\delta p\} = \{R\} \quad (2-38)$$

which is solved symbolically by

$$\{\delta p\} = [C]^{-1}\{R\} \quad (2-39)$$

A similar method is used to solve for $\{\delta T\}$, followed by $\{\delta C\}$. One complete outer iteration [ITNN] in the solution requires one complete pass of solving for $\{\delta p\}$, $\{\delta T\}$, and $\{\delta C\}$. The minimum and maximum number of iterations are set by [MINITN] and [MAXITN].

The solving process, designated by equation (2-39), is accomplished by one of three methods. For a one-dimensional problem, the coefficient matrix C is tridiagonal and is solved directly by the Thomas algorithm (Thomas, 1949; Bennett, 1976). For two- and three-dimensional problems, an option of an iterative two-line successive overrelaxation, or reordered Gaussian elimination method (Price and Coats, 1973) is provided, where the latter is most reliable.

Since the pressure, temperature, and solute equations are coupled by density, large changes in density due to changes in temperature and/or concentration in a grid block may render earlier calculations of pressure, which determines velocities, as inaccurate. Therefore, densities are updated, and the pressure equation is resolved to give new velocities which are inserted in the convective terms in energy and solute equations. A similar process is repeated until the change in density over an iteration is within tolerance limits. For a "difficult" problem, convergence is usually obtained in less than three iterations.

The value of Δt in equations (2-24), (2-25), and (2-26) is either entered or determined automatically. Small user-specified time steps should accompany changes in well flow rates. For sustained runs where no source changes occur, the time step can be determined by the program by using user-

specified maximum allowable changes in pressure, temperature and concentration over a given time step. A new value of time step (Δt^{n+1}) is then calculated based on the previous time step data. Three values of the time step are calculated by using maximum changes in grid block pressure, temperature, and concentration at the previous time step. The following is used for making a pressure estimate of (Δt^{n+1}). Let

δp_s = user-specified absolute maximum pressure change per time step [DPMX],

δp_c = absolute maximum pressure change in all grid blocks at the previous time step [DPMAX],

Δt^n = old time step [DTC],

and

Δt^{n+1} = estimated new time step.

The time step estimation for pressure is predicted by the following:

for $\delta p_c > \delta p_s$

$$\Delta t^{n+1} = \Delta t^n \left(1 + \frac{\delta p_s}{\delta p_c} \right) (.5) ; \quad (2-40)$$

for $\delta p_c < \delta p_s$

$$\Delta t^{n+1} = \Delta t^n \left(.2 + .8 \frac{\delta p_s}{\delta p_c} \right) \quad (2-41)$$

with additional constraints such that

$$\Delta t^{n+1} \leq 1.5 \Delta t^n$$

and

$$\Delta t^{n+1} \leq \Delta t_{\max} \quad [\text{DTMAX}]$$

and

$$\Delta t^{n+1} > \Delta t_{\min} \quad [\text{DTMIN}].$$

The damping factor of .8 in equation (2-41) is used to account for nonlinearities in the linear extrapolation.

INITIAL AND BOUNDARY CONDITIONS

Initial values of temperature and concentration are user specified, either block by block or regionally in the reservoir. The initial pressure is calculated from user specified data of initial pressure [PINIT] at depth [HINIT], density ($\rho(p,T,C)$), elevation, and initial flow field in the reservoir. Temperature can also be specified as a function of depth in the overburden, underburden and aquifer. This option allows one to initialize a geothermal gradient. Regional input of initial temperature is not permitted in the overburden and underburden layers. An example of a common initial condition is

$$p = p_0(z)$$

$$T = T_0$$

$$C_0 = 0$$

and

$$(\cdot)^{n+1} = (\cdot)^n + \delta(\cdot).$$

where $p_0(0)$ is a constant pressure evaluated at the upper-most grid-block in a level reservoir, and T_0 and C_0 equal zero are constant initial temperature, and concentration in all the grid blocks.

The assigned locations of the initial pressure, temperature, and concentrations are located at the top center of each grid block (see Figure 2-1-B); however, the calculated $\delta(\cdot)$ values are calculated at the grid block centers. This discrepancy becomes small when Δz_k becomes small. Similarly, the "best point" location of a source is located at the top center of a cell. Therefore, the new values of pressure, temperature, and concentration are located at the top of the cell as indicated by the update formula of

$$(\cdot)^{n+1} = (\cdot)^n + \delta(\cdot).$$

The program has a number of exterior boundary conditions designated as aquifer influence functions. Each aquifer influence option attempts to model an infinite aquifer (reservoir) without using an infinite or very large grid field. These extensions to an infinite aquifer are necessary because the storativity $\frac{\partial \rho}{\partial p} \bigg|_{T,C} \phi^n + \rho^{n+1} \phi_0 C_R$ due to fluid and rock matrix compression are small, hence the pressure effects travel quickly throughout a solution domain.

The best representation of an infinite aquifer is the Carter-Tracy method (Van Everdingen and Hurst, 1949; Carter and Tracy, 1960). The steady state method (Schilthuis, 1936) is best when a natural flow field is maintained in the reservoir. The "pot aquifer" option, which is the simplest, appears to be least accurate. Details about each of the aquifer influence functions are provided for the user in Appendix B.

The best mathematical representation of these boundary conditions is

$$\lim_{x \rightarrow \infty} p = p_0 \quad (2-42)$$

where p_0 is initial pressure and x is some distance far away from the region of interest.

Temperature and solute fronts travel at a slow rate and are represented by boundary conditions at the edge of the finite difference mesh at $x=L$, where L is sufficiently large and written as

$$\text{at } x = L, T = T_0 \text{ or } \frac{\partial T}{\partial x} = 0, \text{ and} \quad (2-43)$$

$$\text{at } x = L, C = C_0 \text{ or } \frac{\partial C}{\partial x} = 0 \quad (2-44)$$

where T_0 = initial temperature [TWI], and C_0 = initial concentration [SWI], each evaluated at the boundary.

The conditions used depend upon the flow direction. If the fluid mass flow rate (q_w) is out of the finite difference boundary block, the energy ($\dot{q}$) and solute (q_C) loss rates are written as

$$-\dot{q} = -Hq_w$$

and

$$-q_C = -Cq_w$$

where H and C are the enthalpy and concentration at the boundary block, respectively; however, if the fluid mass flow rate (q_w) is entering the boundary block from the exterior, the energy and solute in are evaluated as

$$\dot{q} = H_0 q_w$$

and

$$q_C = C_0 q_w$$

where H_0 and C_0 are the initial enthalpy and concentration, respectively. Therefore, the finite difference domain should be sufficiently large to contain all the injected fluid if any type of recovery simulation is attempted. The contribution of energy and solute transport by dispersion and diffusion across the boundary is assumed to be zero or negligible in comparison to convection transport.

Wells are either sources or sinks where fluid is allocated on a layer by layer basis. If x is defined as a spatial coordinate measured from the well, the source and sink boundary conditions are best described as

$$\lim_{x \rightarrow 0} x \frac{\partial p}{\partial x} = \frac{Q_i \mu}{2\pi k_s \Delta z} \quad (2-45)$$

$$\lim_{x \rightarrow 0} (u\rho C)_i = u\rho C - \rho E_C \frac{\partial C}{\partial x} \quad (2-46)$$

and

$$\lim_{x \rightarrow 0} (u\rho C_p T)_i = u\rho C_p T - E_H \frac{\partial T}{\partial x} \quad (2-47)$$

where $x = 0$ is the location of the source (or sink), uC and $u\rho C_p T$ represent convective transport in x -direction at velocity u , and $\rho E_C \partial C / \partial x$, $E_H \partial T / \partial x$ represents the "total" dispersive flux in the same direction. The variable k_s is the effective permeability ($d(L^2)$) immediately around the borehole, Δz is the vertical length of the well opening, and Q_i is the volumetric flow rate ($d(L^3 t^{-1})$). Equations (2-46) and (2-47) basically indicate that net flux in by source (i) equals net convective flux out plus net "total" dispersive flux out.

Conduction heat losses are allowed through the overburden and underburden blocks. These blocks are treated as semi-infinite rock strata in the z-direction which are devoid of fluid movement; hence, heat is transferred via molecular process. The model assumes one dimensional unsteady heat transfer by conduction normal to the upper and lower reservoir boundaries described by

$$K_{ob} \frac{\partial^2 T}{\partial z^2} = (\rho C_p)_{ob} \frac{\partial T}{\partial t} \quad (2-48)$$

where K_{ob} [KOB] is the effective thermal conductivity and $(\rho C_p)_{ob}$ [CPOB] is the effective specific heat of the overburden. The same equation with different input data ([KUB], [CPUB]) is used for the underburden layer. Initial and boundary conditions for equation (2-48) are

$$T(x_r, y_r, z, 0) = T_0(z) \quad (2-49)$$

$$T(x_r, y_r, 0, t) = T_r(x, y, 0, t) \quad (2-50)$$

and

$$T(x_r, y_r, \infty, t) = T_0(\infty) \quad (2-51)$$

where x_r, y_r are used to specify x and y based on reservoir plane coordinates. In other words, equation (2-49) indicates that initial temperature is a function of depth, equation (2-50) indicates that the lower boundary temperature is the same as the last upper node of the reservoir, and equation (2-51) specifies that the uppermost temperature in the overburden remains constant. Identical boundary conditions also apply to the underburden layer. If the reservoir is only one block thick ([NZ] = 1), the total heat loss is calculated as twice the heat loss to the overburden.

The above method of handling heat transfer is justified when the overall horizontal temperature gradient in the aquifer is small. This is generally true in most problems except near the thermal front; hence, the Peclet number (ratio of convective to conductive transport) is high, and heat conduction in the longitudinal direction can be ignored (Chase and O'Dell, 1973; Coats, George, and Marcum, 1974). This simplification allows a decrease in overall computer storage and computation time because equation (2-48) can be solved directly by the Thomas algorithm (Thomas, 1949). Therefore, heat loss rate through block $\Delta x_i \Delta y_j$ is

$$\dot{q} = \frac{K_{ob}}{\Delta z_0^*} (T_u - T_0') \Delta x_i \Delta z_j \quad (2-52)$$

where nomenclature is given in Figure 2-2.

When using the conduction heat loss option, one should consider Figure 2-2 where the upper and lower reservoir boundaries are shaded. Since the temperature in the reservoir is calculated at the top-center of each grid block in the reservoir, the boundary condition designated by equation (2-50) for the overburden block is $T_u = T_r(x, y, 0, t)$. Such is not the case with the underburden blocks where the equivalent of equation (2-50) is assigned T_L , which is located a distance Δz_3 away from the underburden boundary, as shown in Figure 2-2. The accuracy of heat loss calculations to the underburden blocks can be increased by making Δz_3 smaller, especially if free convection causes the injection fluid plume to drop to the bottom of the reservoir.

Figure 2-2. Temperature assignments to overburden and underburden blocks

WELLBORE MODEL

The wellbore model allows the user to specify surface conditions; hence, bottom-hole pressure and temperature can be unknown. For an injection well, the temperature of the injection fluid [TINJ] is always specified. Two general solution modes are allowed for an injection well and production well. These include a specified injection flow rate, where the bottom-hole pressure is determined from reservoir grid block pressure and injection rate, and the unknown surface pressure at the well-head is obtained by an iterative solution. In the second mode, a limiting surface pressure is specified, and the rate is calculated from surface pressure and bottom-hole grid block pressure by an iterative method. For a production well with flow rates specified, the solution can be obtained directly since bottom-hole grid block pressure and temperature are known and the resultant wellbore solution proceeds from down-hole conditions to the surface. In the second mode, limiting surface pressure is specified; hence, an iterative solution procedure is required to obtain the production flow rate. In actual use, when surface pressure is specified for both injection and production wells, an accompanying flow rate is specified. The program will select either specified flow rate or specified limiting pressure in such a way that one will not exceed the other.

Assumptions used in the wellbore model are

1. fluid flow is steady and incompressible with head losses determined by the flow rate and pipe friction factor and with viscous dissipation neglected in heat transfer segment of the model;
2. initial ground temperatures surrounding each well are known and are expressed as a function of depth $T_{\infty}(z)$
3. heat transfer calculations about the wellbore are transient. The wellbore is treated as a constant line source in an infinite media having thermal diffusivity, $\alpha = K_m / (\rho C_p)_m$ [TDIS] and $K_m =$

$.7071 (K_x^2 + K_y^2)^{1/2}$ where K_x = x-direction thermal conductivity [UKTX] and K_y = y-direction thermal conductivity

[UKTY];

4. fluid properties (viscosity (μ), and density (ρ)) are allowed to vary with pressure and temperature in the wellbore. Fluid properties and friction head losses are constant in a given solution increment (Δz_i) and
5. enthalpy of injection fluid is the same as pure water at the same temperature and pressure. This assumption is good when injected fluid is a solution dominated by water.

The solution method utilizes user-defined depth increments (Δz_i) corresponding to user input of Δp [DELPW], where

$$\Delta z_i = \frac{g_c \Delta p}{(\rho g)_i} = \frac{[\text{DELPW}]}{(\rho g)_i} g_c$$

in which i represents an increment. For production and injection wells, increment count increase from bottom to top, and top to bottom, respectively (Figure 2-3).

Pressure and temperature values are obtained at each end of an increment (Δz_i) by solving a total energy equation simultaneously with an equation of mechanical energy. Total energy balance over an increment (Δz_i) for incompressible fluid flow is

$$\Delta H_i - \frac{g \Delta z_i}{g_c J} = \Delta \dot{Q}_i \quad (2-53)$$

(Change in (Change in (Change in
Enthalpy) Potential Energy) Energy in Fluid)

The heat loss to surrounding media over a length (Δz_i) is

$$-\Delta \dot{Q}_i = \frac{2\pi r_1 K_H \Delta z_i}{q_w} (\tilde{T}_i - \tilde{T}_{R_i}) \quad (2-54)$$

for early time ($4\alpha t / (r_1^2) < 2$) and for later time is

$$-\Delta \dot{Q}_i = \frac{2\pi r_1 K_H K_m \Delta z_i}{[K_m + r_1 K_H f(t)] q_w} (\tilde{T}_i - \tilde{T}_{R_i}) \quad (2-55)$$

$$\alpha = \frac{k_m}{(\rho L \rho)_m}$$

$$= [TDIS]$$

Figure 2-3. Wellbore data definition. Part A shows input data definitions and solution increments, and Part B is a section of a generalized wellbore consisting of the inner tubing and outer casing.

where r_1 = inner radius of wellbore, K_H = heat transfer coefficient through the casing, q_w = fluid mass flow rate through the well, $\bar{T}_i$ = mean temperature of fluid in increment, $\bar{T}_{Ri}$ = mean initial temperature of rocks around the wellbore, and

$$f(t) = -\ln\left(-\frac{r_0}{2\sqrt{\alpha t}}\right) - .290 \quad (2-56)$$

in which α = thermal diffusivity of the rock surrounding the wellbore, t = time elapsed since the start of simulation, and r_0 is the outermost radius of the wellbore. At small t , equation (2-56) is negative and is taken as zero; hence, equation (2-55) reduces to equation (2-54).

Since enthalpy is a function of pressure and temperature, an equation of motion for fluid flow (equation of mechanical energy) is solved to compute pressure as a sum of gravity head and pipe frictional pressure drop as

$$-[\text{DELPW}] = -\Delta p_i = \frac{\Delta z_i \rho_i g}{g_c} + \frac{(\text{fr})_i \rho_i w^2}{4g_c r_1} (\Delta z_i) \quad (2-57)$$

where Δz_i is positive downward, w is the flow velocity in the wellbore and $(\text{fr})_i$ is the pipe friction factor. The value of $(\text{fr})_i$ is determined from the pipe Reynolds number (Re)

$$\text{Re} = \frac{2\rho_i w_i r_1}{\mu_i}$$

and ratio of pipe roughness to diameter

$$\frac{\epsilon}{2r_1} = \frac{[\text{ED}]}{2r_1}$$

where

$$(\text{fr})_i = f(\text{Re}_i, \frac{\epsilon}{2r_1})$$

adapted from the pipe friction factor Moody diagram.

The solution method for each Δz_i (positive downward) uses an iterative technique which starts by estimating ΔH and Δp by equations (2-53), (2-54) or (2-55) and

$$\Delta p_i = \frac{\Delta z_i^{\ell} \rho_i^{\ell} g}{g_c} \quad (\ell = 1).$$

The new enthalpy for the next increment (i) is

$$H_i^{\ell+1} = H_{i-1} + \Delta H_i^{\ell+1}.$$

The average of the new estimated ($H_i^{\ell+1}$) and established old enthalpy at the previous increment (H_{i-1}) is used to calculate the new temperature which is then used to update density and viscosity. A new downstream increment $\Delta z_i^{\ell+1}$ is computed by equation (2-57) using updated fluid properties corresponding to user defined [DELPW]. Convergence is satisfied when

$$\Delta z_i^{\ell+1} - \Delta z_i^{\ell} \leq .5 \quad (\text{ft}).$$

Otherwise, ΔH is recalculated with updated new $\Delta z_i^{\ell+1}$ corresponding to user-specified pressure increment [DELPW]. If convergence is satisfied, calculation proceeds to a new increment (Δz_{i+1}) located uphole or downhole from the previous location in a production or injection well, respectively. The pressure and temperature at the end of the last increment is determined by linear interpolation of the second and third to the last full increment of pressure and temperature calculations.

In a complex wellbore such as that shown in Figure 2-3-B, the coefficient K_H [UCOEFF] is calculated by assuming a standard series resistance method, giving

$$\frac{1}{K_H} = \frac{1}{h} + \frac{r_1 \ln(\frac{r_2}{r_1})}{K_t} + \frac{r_1 \ln(\frac{r_3}{r_2})}{K_s} + \frac{r_1 \ln(\frac{r_4}{r_3})}{K_c} \quad (2-58)$$

where h is the convective heat transfer coefficient between fluid and casing. The K and r represent thermal conductivities and radii of various parts of the wellbore.

The convective heat transfer coefficient is determined by the Nusselt number (Colburn, 1933; Karlekar and Desmond, 1977) as follows:

$$Nu = \frac{hr_1}{K_w} = .023 Re^{.8} Pr^{1/3} \quad (2-59)$$

where K_w = thermal conductivity of the fluid, Re = pipe Reynolds number, and Pr = Prandtl number defined as

$$Pr = \frac{C_p \mu}{K_w} \quad (2-60)$$

Equation (2-59) is good for fully developed turbulent flow, which applies to most problems.

The use of the heat loss wellbore model is most accurate when the input fluid mass flow rate and temperature (production or injection) are constant over a long period of time (see Ramey, 1962). The use of this wellbore model for both injection and production in a single simulation appears questionable because information about temperature changes in the rock matrix due to a previous simulation sequence are not considered in the calculation. This is clear in the derivation of equations (2-55) and (2-56) as shown in Appendix B.

PROGRAM STRUCTURE

The INTERCOMP program is designed so that the redimensioning effort for different problems is kept to a minimum. All data are stored in a single common block. The common block has two regions: one where the length of the common block is fixed for almost every problem, and a second where the size varies from problem to problem. The variable length segment consists of the [G(.)] and [GD(.)] arrays which are partitioned into segments and passed through as arguments in subroutines. The first part is passed as common statements to the subroutines. The [GD(.)] array carries the double-precision array variables.

For most problems, only the array length of the [G(.)] and [GD(.)] segments have to be changed, requiring recompilation of the MAIN program only. This method assumes that the remaining subroutines are compiled previously and retained as an object code. The MAIN program is recompiled after changing the size of [G(.)] and [GD(.)], linked with the remaining object code, and stored as a load module. This simplified data structure allows for easy dumping of restart files.

The program has internal array length calculations, and since all data are stored as two segments in a common block, writing to an external file requires two write statements in addition to knowing the length of each segment. (Actually only one write statement is required; however, INTERCOMP chose to use two). In the modified version, four write statements are used to create the restart files.

Partitioned segments of the main array are called by knowing the location of the first data position, and others follow in designated order. For example, the call statement has a form of

```
[CALL ITER(G(IJPS), G(IKPS), G(IAAQ, ... , G(IPWI), ...)]
```

and the subroutine statement has a form of

```
[SUBROUTINE ITER(JPOS, KPOS, AAQ, ... , PWI, ...)]
```

where [JPOS] and [KPOS] are integer position coefficients, [AAQ] is a constant used to calculate explicit fluid influx across the external boundary, and [PWI] represents the initial node pressure values along the boundary.

The position coefficients are calculated by

$$[JPOS(J) = (J-1) * NX]$$

$$[KPOS(K) = (K-1) * NXY]$$

where [NX] = number of x-direction nodes, and [NXY] = product of number of x and y nodes.

The array position is related to the node position by

$$[M = JPOS(J) + KPOS(K) + 1]$$

where [I, J,] and [K] are counters for x, y, and z node numbers and [M] is the array position.

MAIN PROGRAM

The MAIN program serves as the operating skeleton of the DWDM. The basic components of the MAIN program are given in Figure 2-4. It starts by reading and using the M series of input (Appendix D) to compute individual array lengths in the variable common block to determine the total core size required in the program. For an IBM machine, the last core block position should be less than the allocated size of core in the statement

```
[COMMON DUMMY, GD(2000), G(10000)];
```

that is, the length of the single-precision array [G] and the double-precision array [GD] should be printed as less than 10000 and 2000, respectively. The size of the working array for [GAUS3D] is also approximated in the MAIN program. This value should be greater than the value determined later by subroutine [ORDER] if [GAUS3D] is used in solving equation (2-38).

Restarts of the program are initiated by indicating the time step number [ITIME] desired and having a restart record corresponding to [ITIME] on tape (disk) unit (4) and an output tape (disk) on unit (8). The program then checks to see when the next recurrent data are to be read [TMCHG]. If the time [TMCHG] is less than or equal to current time corresponding to [ITIME], then a new set of recurrent input data are read. Otherwise, execution continues without new recurrent data entry.

In addition to the MAIN program flow path, there are two auxiliary paths for plotting previous run simulation results and mapping output tables from restart records. Data for plots of time vs. pressure, temperature, and concentration are written out to an external storage (tape or disk on unit 12) at every time step [ITIME] in [PRINT2]. The output file is in

```
[FORMAT(2I3,5F10.2,F10.4)]
```

and contains well number, type of well, time in days, bottom-hole pressure (psi), well head pressure (psi), bottom-hole temperature (°F), surface temperature (°F), and solute concentration, in that order. The type of well is coded as

I2 = 1	observation well
I2 = 2	injection well, bottom-hole conditions specified
I2 = 3	injection well, surface conditions specified
I2 = 4	production well, bottom-hole conditions specified
I2 = 5	production well, surface conditions specified.

Data from unit (12) are recalled for plots at the end of a simulation or at a later time. If plots are desired for a previous run, input data must be available on unit 12. Similarly, observed data are also called for if comparison plots are desired. Maps from restart data are handled in a similar manner as restarting the program where restart records at a given time [ITIME] should be available on unit (4). Output to unit (8) is not required. Map format data are read in [READ2], and the contour maps are set-up in [PRINT2] by invoking [MAP2D]. In this mode, flags are set-up to bypass all steps in [READ2] and [PRINT2] that are not associated with restart file mapping. Condition statements for Figure 2-4 are as follows:

1. Are plots desired for a previous run?
2. Is this a restart run?
3. Call [ORDER] if it is not a one-dimensional grid system and if the method of solution is a reduced band width direct solution.
4. Are wellbore calculations to be performed?
5. Is the run to be terminated at this time step?
6. Are wellbore calculations to be performed and is the well rate calculated semi-implicitly?
7. Are any two-dimensional contour maps desired?
8. Are the recurrent data read at this time step?
9. Are any plots desired for this run?
10. Call [ORDER] if it is not a one-dimensional grid and if the method of solution is a reduced band width direction solution.
11. Is the current time [TIME] corresponding to time step [ITIME] less than the time that the next recurrent data are entered [TMCHG]?
12. Are maps desired from previous run restart records?
13. Is the last map from restart records printed?

Figure 2-4. Operating structure of the INTERCOMP DWDM. MAIN program serves as the operating skeleton for the DWDM. (Modified from Figure 2 in INTERCOMP, 1976)

SUBROUTINES

This section is composed of a summary of subprograms in the INTERCOMP code. The basic program structure is given in Figure 2-4. Three major subroutines are called only once before the first time step in each simulation. These are described as follows:

- [READ1] Initial and fixed data are read in this subroutine. These data include all data containing READ R1 series input in Appendix D. Grid block size, pore volume, depth parameters, preliminary fluid flow, thermal conduction in overburden and underburden block transmissibilities, and aquifer influence function coefficients are produced in this subroutine. In addition, subroutines for setting-up viscosity parameters are invoked from this subroutine. Input data are checked for errors as data are entered.
- [INIT] Initial conditions data are read in and checked for errors in this subroutine. Concentration and temperature are initialized according to user specifications for the reservoir. Temperatures in the overburden and underburden are only allowed to vary according to depth. Pressures are computed from the user specified base pressure and the density model using initial concentration and temperature data in the domain. Initial flow velocity in the x-direction is established by use of aquifer influence functions by initial pressure adjustment.
- [PRINT1] This subroutine computes initial fluid in place, initial energy in place, and initial solute in place, and prints out initial grid block value tables.

The next set of major subroutines is called periodically. These are

- [READ2] This subroutine reads in recurrent data which include all data entered as READ R-2 series in Appendix D. Data entered in this subroutine can be altered at any subsequent time specified, thus permitting the user to change well flow rates, temperature and concentration, well specification, time step, differencing scheme, and method of solution. This subroutine also reads parameters to change the tables of output summary. Like [READ1], input data are checked for errors before proceeding. A complete set of data for all options used must be inserted when this routine is called for the first time. Subsequent passes require only changes to the original input.

[COEFF]

Automatic time step is computed when the user specifies and when [ITIME] is greater than one. Overburden and underburden finite difference heat loss calculations assuming no temperature change at the reservoir boundaries are computed, and the coefficient for additional heat loss due to a change in temperature (δT) is evaluated. Viscosities, densities, and enthalpies at each grid block at the old time level (n) are computed. Flow velocities and convective terms ($\rho q_w H$ and $\rho q_w C$)

are weighted according to chosen differencing schemes (central or upwind) and are set up and stored in the residual terms [RW, RH, RC] based on the old time step. Total thermal dispersivity (hydrodynamic plus diffusion) and total solute dispersivity are evaluated and added to proper residual terms [RW, RH, RC]. Tables of Darcy velocities and transmissibilities can be printed if the user wishes at the culmination of this subroutine.

[PROD]

This subroutine calculates rates of injection (or production) into (or from) each layer for each well. The means of allocation uses old time step (n) information. The details on options and means of allocation are given in Appendix C. For the surface conditions specified [ISURF] = 1, the wellbore model [WELLB] is called. Residual terms representing convection and total dispersivity (hydrodynamic dispersion and diffusion) at the old time level n are incremented or decremented by injection or production rates, respectively.

[WELLB]

This subroutine is involved when [ISURF] = 1. It relates surface pressure and temperature to bottom-hole pressure and temperature. Calculations in this subroutine take place over a number of user-specified depth increments based on pressure [DELPW], using an iterative procedure. Net pressure drop consists of a change in gravity head and viscous head loss where the latter is usually small for single phase flow. Enthalpy-in minus enthalpy-out equal to change in internal energy is applied to each increment. Since the last increment may not correspond to a length computed by model, the final pressure and temperature are determined by linear interpolation based on the last two full length increments. For a production well, solution proceeds from bottom-hole to top-hole, and from top-hole to bottom-hole for an injection well. Details on the heat loss calculations in this model are given in the description of the wellbore model and in Appendix B.

[ITER]

This subroutine begins by setting up the coefficients for the aquifer influence functions by expressing the rate of water influx (or efflux) across the boundary as

$$e_w^{n+1} = a + b \delta p \quad (2-64)$$

where a, [AAQ] is the influx based on no change in pressure over a time step (explicit), and b, [BAQ] is a constant which

relates change in pressure δp to an additional influx (or efflux). Coefficient b is added to the proper diagonal element in $[C]$ in equation (2-38).

The primary objective of the subprogram is to solve the vector equations in the following order:

$$[C_3] \quad \{\delta p\} = \{R_3\} \quad (2-65)$$

$$[C_2] \quad \{\delta T\} = \{R_2\} \quad (2-66)$$

$$[C_1] \quad \{\delta C\} = \{R_1\} \quad (2-67)$$

and begins by setting up the coefficient matrix $[C_3]$ and column vector of residuals $\{R_3\}$. The "solving" process in equation (2-39) is accomplished in subroutines $[GAUS1D]$, $[GAUS3D]$, or $[L2SOR]$. A solution is said to have converged when the maximum change in density over all the grid blocks is below a tolerance limit. Included in the iteration process is a means of updating the explicit flow rate in equation (2-32) so that desired well rates are achieved regardless of the change in pressure in the grid block. This adjustment is invoked after the pressure equation is solved. If the new achieved rate after the pressure calculation is not within 5% of old allocated flow rate, the explicit part of the well flow rate to each layer is updated by a ratio of old allocated to new achieved rate (see Appendix C). After an update, the pressure equation is solved again with a maximum of three iterative $[ITRN]$ passes through the pressure equation to adjust explicit flow rates.

The operations flow chart in subroutine $[ITER]$ is given in Figure 2-5. Further operations with $[ITER]$ are reviewed in discussions of subroutines involved in setting up the coefficient matrices and the column vectors for equations (2-65), (2-66), and (2-67).

Condition statements for Figure 2-5 are as follows:

1. Is this the first iteration?

2. Are the cross-derivative dispersion terms to be included?
3. Is the grid block system one-dimensional?
4. Is a direct solution desired?
5. Has convergence been achieved?

[WTFNC] Velocities may change sign because of a change in pressure. INTERCOMP assumes that velocity will not change much over an iteration so [WTFNC] is called only twice during the first iteration. New velocity is evaluated as a sum of old velocity at the previous time step plus velocity change due to δp . Values of [AX] are as follows:

$$\begin{aligned} q \geq 0, \text{ upwind differencing } [AX] &= 0 \\ q < 0, \text{ upwind differencing } [AX] &= 1 \end{aligned}$$

and $[AX] = \Delta x_i / (\Delta x_i + \Delta x_{i-1}) \approx 1/2$ for central differencing. For y and z directions, weighting functions are [AY] and [AZ], respectively. The [AX], [AY], and [AZ] are used in the same capacity as α in equation (2-28-g), but instead of operating on grid block values, [AX], [AY], and [AZ] apply to changes in grid block values as

$$\delta C_{i-\frac{1}{2}} = \alpha^* \delta C_{i-1} + (1 - \alpha^*) \delta C_i$$

in subroutines [SRHA] and [SRHS] where α^* represents a weight function [AX], [AY], or [AZ].

[SCOEF] Coefficients for $[C_{33}']$, $[C_{34}']$, and $[C_{35}]$ in equation (2-36-a) are set up in this subroutine which is called once for each equation. When the pressure solution invokes [SCOEF], all coefficients from $[C_{11}]$ to $[C_{24}]$ are solved as part of solving for $[C_{33}']$, $[C_{34}']$, and $[C_{35}]$. Therefore, after the pressure equation is solved, this routine is called again to solve for intermediate components $[C_{22}']$, $[C_{23}']$, and $[C_{24}]$ for temperature solution and $[C_{11}]$, $[C_{12}]$, and $[C_{13}]$ for contaminant solution. Each time the routine progresses only far enough to evaluate the needed right and left-hand members of [C] and [G] in equation (2-36-a).

[SRHA] This subroutine solves for the update component of the column vector {H} in equation (2-36-a). Implicit components on the right side of equation (2-36-a) are updated and tabulated in this routine.

[CRSS] Cross terms given in equation (2-28-k) are evaluated using the most current updated pressure, temperature, and solute concentration data from the previous iteration.

Figure 2-5. Solution scheme arrangement in subroutine [ITER]. (Modified from INTERCOMP, 1976)

After this set of subroutines is called in [ITER], the coefficient matrix $[C_3]$ and residual column vector $\{R_3\}$ in equation (2-65) are constructed in [ITER]. Implicit components on the right-hand side of equation (2-36-a) are moved to the left side to $[C_3]$ and the remaining column vector is $\{R_3\}$.

[GAUS1D] This is the direct solution solver of equations (2-65), (2-66), or (2-67) if the problem is one-dimensional in x-direction. The Thomas Algorithm (Thomas, 1949) is used to obtain a direct solution for a one-dimensional problem because the diagonal band width in the coefficient matrix $[C]$ is three.

[GAUS3D] This subroutine contains a direct solution algorithm for equations (2-65), (2-66), or (2-67) in two- or three-dimensional domains. The solution method uses an optimum ordering Gaussian elimination scheme (Price and Coats, 1973) that compares favorably with an iterative two-line successive overrelaxation method for large dimensioned problems.

[L2SOR]
[LSORX]
[LSORY]
[LSORZ] This is the calling subroutine for the iterative solution of two- or three-dimensional problems. The scheme used is like a single-line overrelaxation method. Five diagonal terms are present in a double-line solution rather than the usual two in single-line. One of the [LSORX], [LSORY], or [LSORZ] subroutines is called depending upon the orientation of the optimum line.

[SRHS] This subroutine has a similar purpose to [SRHA]. It computes the updated right hand side components for equation (2-36-a) and sets up the implicit components for the coefficient matrix. This subroutine has two parts. One part is called when the temperature solution is activated, and the second part is called when the solute equation is being solved.

As explained in the pressure equation solution, the coefficient matrices for temperature and solute equations $[C_2]$ and $[C_1]$, respectively, are assembled in [ITER] immediately after subroutine [SRHS]. Similarly, $\{R_2\}$ and $\{R_1\}$ are assembled in the same location for the temperature and contaminant equations, respectively. One count of an iteration [ITNN] refers to a passage through all solved equations. Grid block values are updated when convergence is satisfied. This constitutes the end of the solving process in subroutine [ITER].

In the following section, the reader is referred back to Figure 2-4.

After [ITER], [PRINT2] is called to update source terms and print simulation results.

[PRINT2] This subroutine updates the water influx (efflux), energy, and concentration via aquifer influence function blocks. It computes heat loss, water in place, energy in place, and solute mass in place. Tabulations and updates of source rates and wellbore model results are computed in this subroutine in preparation for output tables. Water mass, energy and solute mass balances are performed. Overburden and underburden temperature profiles are updated. Output tables of cumulative flow through wells and aquifer influence functions are printed according to user preference. Output tables of reservoir grid block results are printed for concentration, temperature, and pressure. Output tables of overburden and underburden temperature are also permitted. An output summary of well data is written to unit (12) at the culmination of every time step. Printer maps are also invoked in this subroutine.

[MAP2D] This subroutine prepares printer-plotter maps having up to twenty contour intervals of pressure, temperature and solute concentration. A choice of rectangular cartesian (x,y,z), cylindrical (r,z), cartesian section (x,z), and areal (x,y) maps can be selected at a given time. Three-dimensional (x,y,z) maps are printed as a series of x,y maps for each z layer. Specific contour characters are defined by bilinear interpolation between the four nearest grid block points. The map domain dimensions are defined by the distance between the first and last grid points of the mapped domain rather than the distance between outer-most grid blocks of a domain. Map scale is arbitrary and user specified and may be different in each of the two dimensions. This version of the [MAP2D] program assumes a printer with the capability of ten characters per horizontal inch, six characters per vertical inch, and a minimum page width of 120 characters. Instructions for modification of the above are given in the comment statements in the code. Maps that extend laterally to more than one page length are continued on the next page.

[PLOT]
[TSHIFT]
[YAVG] These subprograms are invoked by the MAIN program. Program [PLOT] calls two short subroutines [TSHIFT] and [YAVG] in the creation of plot files. It plots pressure, temperature, or concentration vs. time at any specified well and also plots comparative input data from observations with calculated values of the same variables as a function of time. Results are shown as an x-y plot where two dependent variables (observed and calculated) are plotted against the abscissa value of time. Two characters--x-calculated, O-observed--are used. An additional character * is used for coincident results. The length of the

ordinate (across the page) is set, and the length of the abscissa (down the page) is user-specified.

The above-paragraphs present a list of major subroutines. The remaining group of supporting subprograms which were not discussed above are listed below.

- [INITL] This subroutine loads user-specified initial temperature and solute concentration by the region to grid blocks. It is called by subroutine [INIT] as part of the initializing process.
- [ERRPRT] This subroutine prints the output tables of probable input errors in subroutines [READ1], [READ2], and [PRINT1].
- [PRINTS] This subroutine prints the output tables of pressure, temperature, and concentration at the top center of a grid block. The zero pore volume blocks are left as blanks. The entry point [PRINT0] is for printing output tables for overburden and underburden temperature. Tables of grid block parameters are also printed by this routine. The output tables of transmissibilities (2-28) require some clarification. In this regard, figure 2-6 is a simplified one-dimensional grid block problem. Because transmission coefficients are defined at the grid block boundaries, the output table will print

$$0.0 \quad T_2 \quad T_3 \quad T_4 \quad T_5$$

where T_i refers to a transmissibility defined by Figure 2-6.

In the model, for a pressure equation in radial coordinates, the pressure drop between the first node and well is actually determined by the well index evaluated at T_1 (Appendix C). This subroutine is invoked by [READ1], [PRINT2], [COEFF], and [PRINT1].

- [INPUT] This subroutine contains the library for Tables 2-1 and 2-2. It loads the data into proper arrays for future use. This subroutine is called by [READ1].
- [VISL] This subroutine sets up some of the initial parameters for the viscosity model. Constants B_i and B_r in equation (2-15) are computed. The values of B_i or B_r are calculated by input data tables or internal Lewis-Squire data. If the injection reference viscosity temperature [TIR] is not the same as the reference temperature of the reservoir fluid [TRR], the injection temperature fluid reference viscosity is adjusted by equation (2-13). This routine is called once by [READ1].

- [VISM] Once B_i and B_r are known, the viscosity model requires the use of equation (2-14) or the data tables on viscosity vs. concentration at reference temperature to compute $\mu(T_r, C)$ in equation (2-13). All of this occurs in entry point [VISM]. This routine is called by [READ1], [INIT], [COEFF], [READ2], [WELLB], [PRINT2], and [PRINT1].
- [TRANS] This subroutine takes a REAL*8 variable array and makes it a REAL*4 array. It is called by subroutines [PRINT2] and [PRINT1].
- [TCALC] This is a function subprogram designed to compute fluid temperature from grid block enthalpy and pressure using an iterative procedure. It is called by subroutines [PRINT2], [PROD], and [WELLB].
- [DDINT] This is a function subprogram designated by $f_1(T_o)$ in equation (2-17). It is a linear interpolation routine used to determine saturated enthalpy from Table 2-1.
- [TODINIT] This is a function subprogram designated by $f_2(T_o, P_o)$ in (2-17). It is the two-dimensional linear interpolation for deviation from saturation in the enthalpy model. Both [TODINT] and [DDINT] occur together as in equation (2-17). They are called by subroutines [READ1], [PROD], and [TCALC].
- [AMOODY] This function subprogram computes the friction factor for a given pipe Reynolds number and pipe roughness to diameter ratio. This is called by [WELLB].

Figure 2-6. Locations of transmissibility T relative to grid block transmissibility tables printed by [PRINTS].

SELECTION OF SOLUTION, GRID, AND TIME STEP SIZE

This section is a summary of considerations in selecting the solution scheme (direct or iterative), grid block, and time step size. More detailed information can be obtained from INTERCOMP (1976).

For a one-dimensional problem, one direct solution scheme is offered. This solution scheme will be used whether the user specifies a direct or iterative solution (see Figure 2-5).

In multi-dimensional problems, the user is offered a choice of an iterative solution by two-line successive overrelaxation [L2SOR] or a reord-ered Gaussian elimination direct solution [GAUS3D] (Price and Coats, 1973). Basic experiments by INTERCOMP comparing the two solvers suggest using [L2SOR] when the minimum product of the number of grid blocks in two dimensions is greater than 50 to 75. The iterative solver [L2SOR] has disadvantages because it is an iterative solution subjected to small convergence errors. An obvious sign of such an error in output is the drifting of temperature values outside the thermal front. For a problem having small number of mesh in two dimensions, [GAUS3D] would probably be faster than [L2SOR]; however, the direct solution [GAUS3D] requires more core memory than [L2SOR].

The rate of convergence in an [L2SOR] solution depends upon the choice of an acceleration parameter, ω . The code evaluates ω for the user at specified iteration intervals [IMPG] in the iterative solution. The accuracy of determining the "best" ω increases as the number of iterations increase. The INTERCOMP recommended values of [IMPG] range from three to ten. For highly transient problems, [IMPG] should be set small but it should be larger when domain conditions approach steady-state.

In general, in order to restrict computing expenses one would desire large grid block sizes and large time steps. In general terms, a problem becomes more accurate as

$$\Delta p / \Delta t \text{ approaches } \partial p / \partial t$$

$$\Delta p / \Delta x \text{ approaches } \partial p / \partial x$$

or as Δx , Δt , and Δp become very small. Therefore, the size of the mesh should be finest when the gradient of a quantity (p , T , C) is greatest, and the time step size should be made small when some quantity changes rapidly. Since each equation behaves differently, an ideal mesh and time step for one may not be ideal for the other. A good example of this is a simultaneous solution of the pressure and temperature equations. If a high temperature fluid is being injected, the pressure equation starts by requiring very small time steps because $\partial p / \partial t$ is large at early time because of the small rock and water compressibilities. In contrast, the energy equation shows less rapid changes in temperature with time because of the larger magnitude of the energy storage coefficients between rock and water. The spatial derivatives for this type of problem require similar attention. A fine mesh is required throughout the expected region traversed by the thermal plume because $\partial T / \partial x$ is large at the thermal front and the thermal front is expected to expand in a given domain with time. The mesh size outside the thermal plume region can be set with larger spacing because $\partial p / \partial x$ approaches a small value away from the source of injection. Similar arguments also apply to the density, viscosity, and other derivatives in the governing equations. The DWDM uses the most restrictive time step in the automatic time step routine. Therefore, if pressure is changing most rapidly with time, the time step size will depend upon pressure changes.

The code offers implicit and central in time; and upwind and central differencing in space options on the first derivative in the convective terms in equations (2-3) and (2-4). The pressure equation is unaffected by the above options and is always solved implicitly (in time) and central in space. The advantages and disadvantages of each are discussed below.

For large grid blocks, second-order (proportional to terms having second derivatives) space and time truncation errors originating in the convective and time terms (shown in the left side in equation (2-68)) contribute to physical dispersion. This is shown by writing a one-dimensional simplified version of equations (2-6) and (2-7) as follows:

$$S \xi_t + M u \xi_x = E \xi_{xx}. \quad (2-68)$$

One can show the cause of this error from the simplified one-dimensional form of equations (2-6) and (2-7) where $\xi_t = \partial \xi / \partial t$ in which ξ can be C or

T. Writing equation (2-68) using implicit and upwind differencing and a Taylor series representation of the finite difference derivatives to return to a form of equation (2-68) gives

$$\xi_t + \frac{M}{S} u \xi_x = \frac{E}{S} \xi_{xx} + \frac{u^2 \Delta t}{2} \xi_{xx} + \frac{M}{S} \frac{u \Delta x}{2} \xi_{xx}. \quad (2-69)$$

The additional terms

$$\frac{u^2 \Delta t}{2} \quad (2-69-a)$$

and

$$\frac{M}{S} \frac{u \Delta x}{2} \quad (2-69-b)$$

are second-order terms that contribute to the physical dispersion-diffusion level. The term designated by (2-69-a) is the result of implicit (time) differencing, while the term designated by (2-69-b) is the result of upwind dif-

ferencing on the convective term in equation (2-68). This means the total dispersivity in equation (2-69) is

$$\frac{E}{S} + \frac{u^2 \Delta t}{2} + \frac{M}{S} \frac{u \Delta x}{2}$$

rather than the physical dispersivity of E/S . To prevent numerical diffusion from overcoming physical dispersion-diffusion, the following should hold:

$$\frac{u^2 \Delta t}{2} + \frac{M}{S} \frac{u \Delta x}{2} \ll \frac{E}{S}$$

or, when dropping the physical terms M/S , the following should hold:

$$\frac{u^2 \Delta t}{2} + \frac{u \Delta x}{2} \ll \frac{E}{S} \quad (2-70)$$

This error does not exist in central in space and central in time (Crank-Nicholson) differencing because in both cases the truncation error is other than second-order. If the molecular diffusion (D_m or K_m) is much smaller than hydrodynamic dispersion, the restriction for Crank-Nicholson and upwind in space is

$$\frac{u \Delta x}{2} \ll \alpha_L \tilde{u}$$

or

$$\frac{\Delta x}{2} \ll \alpha_L \quad (2-71)$$

where α_L is the longitudinal dispersivity factor. The value of α_L usually ranges from 10m (30 ft) to 30m (100 ft); hence, equation (2-71) can be a severe limitation.

Central difference space and time is theoretically stable; however, solutions are sometimes plagued by the tendency of overshooting and undershooting the solution defined by input. For central in space and implicit differencing INTERCOMP recommends

$$\frac{u \Delta x}{2} \leq E_C \quad (2-72)$$

and

$$\frac{u\Delta x}{2} < \frac{E_H}{\rho C_p} \quad (2-73)$$

Similarly, the following are recommended for any Crank-Nicholson differenced problem:

$$\frac{u\Delta t}{2\phi\Delta x} \leq 1. \quad (2-74)$$

The exact adherence to equations (2-72), (2-73), and (2-74) is not necessary to achieve good results. These equations should be used as an estimate to reduce solution oscillation when they are noted. Problems subjected to small oscillation may still yield good results when grid block values are averaged over several time steps. A summary of this section is given in Table 2-3.

The results of this section may be used to minimize solution error. Table 2-3 is good for most problems because most simulations have a dominant Darcy velocity, u in a direction parallel to a length increment Δx , Δy , or Δz . For a radial system, Δx and u can be estimated by:

$$u = \frac{Q}{2\pi r \Delta z} \quad (2-75)$$

and

$$\Delta x = \Delta r = r \Delta \ln(r) \quad (2-76)$$

where r is a grid block boundary and $\Delta \ln(r)$ is the natural logarithmic radius difference between two adjoining grid block centers.

Discussions involving the explicit formulations are not included here because of the restrictions on problem stability, and explicit (time) options are not offered by this code. Additional information and solution improvements can be obtained from Price, Cavendish and Varga (1968), and Lantz (1971), and Roache (1976).

Table 2-3. Summary of Numerical Diffusion and Stability

Difference Form		Numerical*	Stability Consideration
Spatial	Time	Diffusivity	
BIS (upstream)	BIT (implicit)	$u\Delta x/2 + u^2\Delta t/2$	None
CIS (centered)	BIT (implicit)	$u^2\Delta t/2$	$u\Delta x/2 \leq E$
BIS (upstream)	CIT (Crank-Nicholson)	$u\Delta x/2$	$u\Delta t/(2\phi\Delta x) \leq 1$
CIS (centered)	CIT (Crank-Nicholson)	None	Same as above.

CIS--Central in space
 BIS--Backward in space
 CIT--Central in time (Crank-Nicholson)
 BIS--Backward in time (implicit)

*These values reflect only the magnitude of the numerical diffusivity. The actual values have physical constants related to the numerical diffusivity magnitude. (Modified from INTERCOMP, 1976).

SUMMARY

The simulator capabilities are best described by Figure 2-7. Finite difference solutions of pressure, energy, and concentration make up the reservoir model where each equation is dependent upon the other because of fluid viscosity and density. Aquifer influence functions are a means of simulating infinitely large aquifers without infinite finite difference mesh extensions. Conduction heat losses (or gains) are allowed through the overburden and

underburden layers. The wellbore model predicts bottom-hole or surface conditions, depending upon flow direction.

Figure 2-7. Schematic of the simulator (adapted from INTERCOMP, 1976)

PART 3

PROBLEM STATEMENT

PART 3

PROBLEM STATEMENT

INTRODUCTION

This section is composed of a demonstration of code responses between International Business Machine (IBM) and Control Data Corporation (CDC) data mode machines.

Most of the DWDM code development took place on a CDC data mode machine with the intention of operating the code on other machines having less accurate data management format like UNIVAC, IBM, and XEROX SIGMA.

Initial results from several test runs on an IBM-type machine (Amdahl 470V/8) following the code adjustment instructions for IBM data mode gave results that showed significant mass and energy balance errors, whereas CDC results showed perfect mass and energy balance on a few test problems. This error occurs because an IBM data mode machine carries out arithmetic operations to seven places, which is adequate for business transactions. In contrast, CDC carries out similar operations to fifteen places (Table 3-1).

Corrective measures for IBM-type machines required storage of a few single variables and arrays in double precision. The number of these double storage locations were kept to a minimum to minimize the increase in storage and computer time requirements.

Table 3-1. Computer Data Characteristics

(Adapted from Hughes, Pfleeger and Rose, 1978)

Computer Type	Integer Precision (Digits)	Real Range	Real Precision (Digits)	Characters per word
CDC-6000-7000	18	10^{-293} - 10^{+322}	15	10
IBM 360-370	9	10^{-78} - 10^{+75}	7	4
UNIVAC 1108-1110	10	10^{-38} - 10^{+38}	8	6
XEROX SIGMA 5-7	9	10^{-78} - 10^{+75}	7	4

TEST RADIAL COORDINATE PROBLEM

To demonstrate the problem, an example documented in the INTERCOMP DWDM is used to show differences in output (Figure 3-1). This problem uses the radial mesh option with a $10 \times 1 \times 5$ (x,y,z or r,y,z) finite difference mesh at a depth of 1219 meters (4000 feet). This encloses an external radius of 1524 meters (5000 feet) with 5 layers of differing characteristics having a total thickness of 30.48 meters (100 feet). The overburden and underburden consists of 3 grid blocks each in the z-direction. The data used are listed in Table 3-2. The wellbore model is set with a specified injection flow rate and surface temperature, but with unknown downhole temperature and pressure. The flow rate is allocated between layers based on mobilities and the implicit pressure drop between the wellbore and the adjoining grid block. The pressure and energy equation are solved for a two-day injection rate of $283.17 \text{ m}^3/\text{day}$ ($10^4 \text{ ft}^3/\text{day}$) followed by a rest period of three days. Viscosity is allowed

to vary as a function of the dependent variables (p, T). Since only reference viscosities are supplied (see Table 3-2), the model uses the internal Lewis Squire viscosity table. Because the aquifer is anisotropic and inhomogeneous, the nonlinear differential equations have no known analytical solution.

Mesh generation is accomplished by an internal routine which satisfies

$$\frac{rc_{i+1}}{rc_i} = C$$

where [RR], rc_{i+1} = radius to center of $i+1^{th}$ block and [RR], rc_i = radius to center of i^{th} block from the center of symmetry. For this demonstration problem, C is 2.27 and the radius to the first block boundary is .11 m (.37 ft).

Comparisons of mass and energy balances for the above problem run on CDC and IBM showed differences in balance results and minor differences at the individual nodes. The resultant node values compared well within three significant digits for pressure, and within two for temperature. However, cumulative terms like total heat loss, total mass, and total energy balance did not match at all time steps. An example of this difference is shown in Figure 3-2 where the energy balances are compared between CDC or fully-double precision codes with unaltered and improved versions of the simulator. Perfect energy balance of 1.0 is obtained on a CDC run. Energy balance errors are obtained when the unimproved version of the code is operated on an IBM type machine for the same problem. The plot of "IBM improved" shows the energy balance after code improvement. The energy balance is defined as

$$[MBQ] = \frac{\dot{Q}_o - \dot{Q}_n + \dot{Q}_g}{\dot{Q}_L} \quad (3-1)$$

when total energy loss is greater than energy gained in the reservoir. Similarly, when energy gain dominates over loss, energy balance is evaluated as

$$[MBQ] = \frac{\dot{Q}_n + \dot{Q}_L - \dot{Q}_o}{\dot{Q}_g} \quad (3-2)$$

where $\dot{Q}_o$ = initial energy in place at the beginning of the simulation [IQIP], $\dot{Q}_n$ = current energy in place [QIP], $\dot{Q}_g$ = total energy gain, and $\dot{Q}_L$ = total energy loss. For a perfect energy balance [MBQ] is equal to one. The significance of equations (3-1) and (3-2) is clear when both are rearranged as follows:

$$[MBQ] \dot{Q}_L - \dot{Q}_g = \dot{Q}_o - \dot{Q}_n \quad (3-3)$$

and

$$[MBQ] \dot{Q}_g - \dot{Q}_L = \dot{Q}_n - \dot{Q}_o \quad (3-4)$$

The computation for fluid and contaminant mass balance is performed in a manner similar to equations (3-1) and (3-2).

The primary cause of what appeared to be a mass and energy balance error was errors in calculating the total values of mass and energy for the domain.

For the radial test problem, the calculations proceed as follows:

pore volume at the M^{th} grid block is calculated by

$$V_{p_{i,k}} = \pi(rb_{i+1}^2 - rb_i^2)\Delta z_k \phi_{i,k} \quad (3-5)$$

and for the cartesian coordinates pore volume is calculated by

$$V_{p_{i,j,k}} = (\Delta x_i \Delta y_j \Delta z_k) \phi_{i,j,k} \quad (3-6)$$

Figure 3-1. Schematic of test comparison problem. Aquifer zone is anisotropic and inhomogeneous $10 \times 1 \times 5$ (x,y,z,) finite difference grid.

Table 3-2. Radial Test Problem Physical Data

Reservoir Data

Water Compressibility	4.35×10^{-10} 1/N/m ²	(3.0×10^{-6} 1/psi)
Rock Compressibility	5.80×10^{-10} 1/N/m ²	(4.0×10^{-6} 1/psi)
Water Thermal Expansion	3.60×10^{-4} 1/°C	(2.0×10^{-4} 1/°F)
Water Heat Capacity	4.21×10^3 J/kg°K	(1.005 Btu/lbm °F)
Rock Specific Heat	1.88×10^6 J/m ³ °K	(28.00 Btu/ft ³ °F)
Thermal Conductivity of Matrix	1.87 W/m°K	(26.00 Btu/(ft day°F))
Longitudinal Dispersivity	30.48m	(100.0 ft)
Transverse Dispersivity	3.05m	(10.0 ft)
Fluid Density	1.13×10^3 kg/m ³	(70.51 lbm/ft ³)

Layer Description

Thickness	K_r (m/day)	K_z (m/day)	ϕ
6.10m (20 ft)	.110 m/day (.360 ft/day)	.037 m/day (.120 ft/day)	.099
3.05 (10.0)	.089 (.291)	.030 (.097)	.097
6.10 (20.0)	.101 (.330)	.034 (.110)	.107
6.10 (20.0)	.146 (.480)	.049 (.160)	.107
9.14 (30.0)	.030 (.099)	.010 (.033)	.096

Inner Radius Grid Block Boundary

Block	Radius (m)	
1	0.116 m	(0.38 ft)
2	0.945	(3.10)
3	2.146	(7.04)
4	4.877	(16.00)
5	11.079	(36.35)
6	25.173	(82.59)
7	57.196	(187.65)
8	129.948	(426.34)
9	295.235	(968.62)
10	670.767	(2200.68)

Heterogeneity Region - Aquifer Modification

Blocks 1 to 3 in x-direction

Blocks 1 to 5 in z-direction

Hydraulic Conductivity - r-direction = $1/2K_r$

Hydraulic Conductivity - z-direction = $1/2K_z$

Time = 0.0 to 2.0 Days

Injection Rate = 283.17 m³/day (10000 ft³/day)

Surface fluid temperature = 23.9 °C (75.0 °F)

Fluid Viscosity = 1.04×10^{-8} N-day/m² (.900 cp)

at temperature = 59.9 °C (139.8 °F)

Geothermal Gradient:

<u>Depth</u>		<u>Temperature</u>	
0.0 m	(0.0 ft)	23.9 °C	(75.00 °F)
1829	(6000.)	78.1	(172.5)

Overburden - Underburden Data

Input Δz		Actual Node Spacing	
6.10 m	20.0 ft	12.19 m	40.0 ft
12.19	40.0	18.29	60.0
24.38	80.0	18.29	60.0

Specific Heat = 1.88×10^6 J/m³ °K (28.0 Btu/ft³-°F)

Thermal Conductivity = 1.87 W/m °K (26.0 Btu/ft-day-°F)

Since rock is assumed to be slightly compressible, the true pore volume after dropping all reference subscripts becomes

$$V_w = V_p (1 - c_R (p - p_0)) \quad (3-7)$$

The density ρ_w at the M^{th} block is calculated by equation (2-12) so that

the mass of the fluid in place at the M^{th} block is

$$Q' = \rho_w V_w$$

and the energy in place is

$$\dot{Q}' = \rho V_w (U_0 + C_p (T - T_0)) + V_R (\rho C_p)_R (T - T_0)$$

where V_R = the constant volume of rock in matrix ($V_t - V_p$). The contaminant in place is computed by

$$Q'_C = \rho V_w C.$$

Equation (2-21) assumes that energy in the fluid is just a function of temperature above a base internal energy which, in turn, is a function of both pressure and temperature ($U_o(p_o, T_o)$) given as

$$\dot{Q}'_w = (\rho V)_w (U_o + (C_p)(T - T_o))$$

Additional energy stored in rock then is

$$\dot{Q}'_R = V_R (\rho C_p)_R (T - T_o)$$

where energy stored in the rock is zero at reference temperature T_o [T_0].

The total mass of fluid, energy, and mass of component is solved for by summing equations (2-22), (2-21), and (2-23) for all grid blocks.

In taking the radial grid problem (see Table 3-2) into consideration with Δz_2 as 3.05 meters (10 ft), and

$$\frac{rc_{i+1}}{rc_i} = 2.27$$

it is immediately seen that the pore volume in the innermost block is of an order of $.85 \text{ m}^3$ (30 ft^3) whereas it is $3.30 \times 10^5 \text{ m}^3$ ($1.20 \times 10^7 \text{ ft}^3$) in the outermost block when assuming a porosity of .10. Fluid mass, energy, and contaminant mass are multiples of the pore volume so the reason for the calcula-

tion error becomes evident in that summing takes place from M equals one to M equals the number of blocks. For the above problem,

$$1 \leq M \leq 10$$

sums from the inner to outer block, along the top row, and

$$11 \leq M \leq 20$$

sums in the same direction along the second row. Consequently, information about inner cell changes is lost when solving equations (2-22), (2-21), and (2-23) for [IQIP] or [QIP] and related components.

This problem is corrected by doubling the precision of calculations rather than changing the summation order, because a different order of summation might be required for certain linear grid problems.

The test problem described above solves only pressure and energy equations; hence, no contaminant solution comparisons are available. Balance corrections to the energy equation also are applied to the solute balance because much of the contaminant balance is handled in the same manner.

The responses in Figure 3-2 need additional explanation. In the above problem, cool surface water of 23.89° C (75° F) is injected into a deep formation having an initial average temperature of 60° C (140° F). At a dimensionless time of .21 (1.06 days), the quantity of heat injected is 4.19×10^{10} Joules (J) (3.97×10^7 Btu). However, the quantity of heat loss through convection transport of water leaving the finite difference reservoir is 9.67×10^9 J (9.17×10^5 Btu) and heat gain via overburden and underburden conduction is 1.45×10^{10} J (1.37×10^7 Btu). Therefore, heat gain dominates so [MBQ] is calculated by equation (3-2) giving [MBQ] = 1.0295 and [MBQ] will remain equal to one in the program output because of an overriding factor used in the code for IBM machines. The energy balance will continue to have a value of one

Figure 3-2. Energy balance on variable grid size problem

until the quantity of energy gain or loss reaches a certain fraction (FR) of the total energy initially in place [IQIP]. For this problem, when data obtained from the modified version of the code are used, the following outputs are observed at $t = 1.06$ days:

$$Q_o = 6.207704 \times 10^{12} \text{ Btu}$$

$$Q_n = 6.207758 \times 10^{12} \text{ Btu}$$

$$Q_L = 9.169420 \times 10^5 \text{ Btu}$$

$$Q_g = 5.334253 \times 10^7 \text{ Btu}$$

where the breakdown of the latter two are

$$(Q_L) - \text{total heat gain} = 3.97 \times 10^7 + 1.37 \times 10^7 = 5.33 \times 10^7 \text{ Btu and}$$

$$(Q_G) - \text{total heat loss} = 9.17 \times 10^3 \text{ Btu caused by fluid efflux.}$$

By equation 3-2,

$$[MBQ] = 1.0295$$

rather than 1.000 as suggested by the program output. The value of one is given because INTERCOMP anticipated mass and energy balance errors when Q_L or Q_G is small compared to initial total energy in place [IQIP]. For the above calculation

$$FR = 6.21 \times 10^7 = IQIP * (\text{correction factor})$$

and because Q_L dominates and

$$Q_L < 6.21 \times 10^7 = FR$$

[MBQ] is assigned a value of one. However, at the next time step at time = .32 (1.56 days)

$$Q_L = 7.81 \times 10^7 > 6.21 \times 10^7 = FR$$

so the true [MBQ] value is assigned. Therefore, it is possible for problems having very large domains to have perfect output mass and energy balance for a long period of time, or until Q_L or Q_G becomes greater than FR.

INTERCOMP assigns correction factors (CR) as follows:

$$\text{CDC} - 1.0 \times 10^{-8},$$

$$\text{UNIVAC} - 1.0 \times 10^{-6}, \text{ and}$$

$$\text{IBM-SIGMA} - 1.0 \times 10^{-5}.$$

where $\text{FR} = \text{CR} * \text{IQIP}$.

In general, mass and energy balances get better as the quantity of mass or energy injected or produced gets larger as a function of time.

This type of error will probably occur in large domain, low grid density, axisymmetric problems using variable grid sizes defined by

$$rc_{i+1}/rc_i = C.$$

To prevent this problem, the mesh size should be entered manually using smaller increases of Δr_i as r increases.

Dependent variable arrays for the reservoir are stored in double precision. This change forces a number of calculations to take place using double-word accuracy, which increases the accuracy of pressure calculations at near equilibrium conditions in deep aquifers. Another reason for this change is to allow higher precision of calculations of parameters (e.g., density) based on a difference between present values of dependent variables and initial or base values.

For example, if $T - T_0$ is small, and $f(T - T_0)$ represents some function which is a multiple of pore volume at the outer edge boundary block of the previously explained problem, a small error in $T - T_0$ can lead to significant errors in property calculations relative to a small inner block.

For the previous problem, the effect of removing the double-precision dependent variable arrays is shown in Figure 3-3. In Figure 3-3, the abbreviation D.P. refers to double precision, and the "IBM improved version"

contains all corrections including double precision dependent variable arrays. The "IBM no D.P. array" contains the previous corrections with single precision dependent variable arrays. The effect of removing all double-precision arrays results in energy balance errors of lesser magnitude than the results obtained from the unimproved code. This shows that only part of the error comes from calculating [IQIP] and [QIP], which require only double-precision calculations around single variables.

If the grid is of uniform size, the mass and energy balance is usually fairly accurate. This is shown in Figure 3-4, where the results are given for a similar problem using cartesian coordinates with uniform mesh size. In Figure 3-4, the abbreviation D.P. refers to double precision, and since the two lines overlies in space, the differences between the two modes are shown numerically, in the left corner. The "IBM improved" and "IBM-improved with no double-precision dependent variable arrays" yield similar energy balances. Similar calculations using the unimproved version of the code also yield near-perfect energy balances.

Another cause of poor substance balance is due to the differences in physical responses of each equation. Pressure changes which accompany system changes occur very rapidly after the onset of a change in the source flow rate. These pressure changes are the result of small values of c_R and a_1 in equation (2-29) and require very small time-steps for solution accuracy at the onset of a source start-up or shut-down. For example, a problem with a high permeability flow domain can be simulated using large spacing because $\partial p / \partial x$ is small; however, the temperature or the concentration calculation is usually inaccurate at early time because the effects of enthalpy and concentration of fluid injected have yet to pass or affect the large first grid

Figure 3-3. Energy balance comparisons using REAL*4 and REAL*8 arrays

Figure 3-4. Energy balance on a problem of uniform grid size

block containing the source. If the grid block is sufficiently large, it may take a number of time steps to see a change in temperature and concentration. In other words, the movement of the concentration front and thermal front are much slower than the movement of the pressure front. This situation may lead to poor balance of energy and solute mass at early time when relatively large grid blocks are used.

The pressure equation approaches steady-state quickly; thus, the required size of the time steps increases to retain the same accuracy for the pressure equation, and the size of the time steps becomes dependent upon changes in solute concentration or temperature in the automatic time step mode. If the magnitude of $\partial C/\partial x$ or $\partial T/\partial x$ remains small, the domain of large grid blocks may be sufficient for an accurate solution; hence, the resultant substance balance gets better with time.

In general, substance balance should approach 1.00 rapidly after code start-up or perturbation. If a substance balance gets progressively worse with additional time steps, something is probably incorrect about the computation.

CODE COMPARISON RESULTS

This study compares responses of three IBM run versions of the code. A fourth output from the radionuclide transport version (version 2) of DWDM run on CDC was also used in the comparison. The problem simulated was discussed in the previous section. The CDC output was obtained from a more advanced version of the code; consequently, some of the basic algorithms in the code may have been slightly altered. The IBM run versions include (a) code without alterations, (b) code with partial alterations discussed in the

previous section, and (c) code with fully double-precision real variables. Code responses documented in this section are the results of using an "older" version of the altered code. This version contained a number of errors involving the use of the geothermal gradient and heat loss calculations. These errors are likewise contained in the other versions compared in this section. For example, the final altered version included with this report predicts a small net heat gain by conduction from overburden and underburden; hence, it cannot reproduce Figure 3-7. Results shown on Figures 3-8 and 3-9 can be closely duplicated by the final altered version.

In general, node point results of all IBM output are nearly identical to CDC results. Pressure values are usually accurate to within the nearest 1.38×10^4 Newtons/m² (N/m²) (2.0 lb/in²) and .56 °C (1.0 °F). The results tend to differ most when a sudden perturbation, such as a change in flow rate or a change in the temperature of the injection fluid is introduced to the simulation. Comparison plots of CDC and partially altered IBM version results show that maximum δp and δT differences approach zero as time proceeds past the initial perturbation (Figures 3-5 and 3-6). The relative magnitude of differences are small, having maximum values 2% of δp and δT at all node points.

In Figure 3-5, time equal to 1.0 corresponds to .426 days after initial perturbation, and dimensionless pressure equal to 1.0 corresponds to 1.04×10^6 N/m² (150. lb/in²). The dp equal to 1.0 corresponds to 1.72×10^4 N/m² (2.5 lb/in²). The squares are IBM results, and the circles are CDC results. The maximum changes occurred at the same node points, with the exception of the second time step ($t = .0469$ days). The maximum change occurred at node 1,1,5 for IBM and 3,1,5 for CDC. The comparison shown is for node 1,1,5.

In Figure 3-6, dimensionless temperature equal to 1.0 corresponds to 3.53°C (6.35°F), and dimensionless time equal to 1.0 corresponds to .426 days. All maximum temperature changes occurred at identical node locations in CDC and IBM calculations.

The largest discrepancy in cumulative numerical values between the partially altered code and CDC occur in the tabulation of cumulative heat loss to the confining rocks followed by cumulative heat loss due to convection out through the periphery of the reservoir (Figures 3-7, 3-8, and 3-9). Figure 3-7 shows the comparisons between improved IBM and CDC predicted heat loss via overburden and underburden conduction. The heat loss calculation by IBM lags behind the CDC results. In Figure 3-7, maximum time is 5.0 days, and maximum heat loss corresponds to $3.09 \times 10^{10}\text{ J}$ ($2.93 \times 10^7\text{ Btu}$). This value is orders of magnitude smaller than total energy in the aquifer of $6.55 \times 10^{15}\text{ J}$ ($6.21 \times 10^{12}\text{ Btu}$). Figures 3-8 and 3-9 are comparisons of fluid and energy efflux at the periphery of the simulated field. In Figure 3-8, the IBM results are squares and CDC results are circles. Results are nearly identical, and maximum time corresponds to five days and maximum fluid efflux to $2.05 \times 10^{-1}\text{ million kg}$ ($4.53 \times 10^{-1}\text{ million lbm}$). Cumulative fluid efflux differs slightly for IBM and CDC computations where cumulative energy efflux for IBM is somewhat less than the CDC computation. In Figure 3-9 response for IBM is delayed slightly, and then displays parallel response; again the quantity of energy efflux is very small compared to the total system because 1.0 in Figure 3-9 corresponds to $5.38 \times 10^{10}\text{ J}$ ($5.10 \times 10^7\text{ Btu}$). For Figure 3-9, the CDC results are circles, and IBM results are squares, with maximum time corresponding to five days. The partially altered IBM version yields results that are nearly identical to the fully double-precision version. However, the

unaltered code shows $\pm 5\%$ difference in heat loss calculation when compared to altered versions during the 5-day simulation.

The effect of the above-mentioned differences contributes to overall mass and energy balances because the magnitude of differences noted are compared to differences of total substance in place at present and total substance in place initially. In general, these discrepancies in the worst case cause [MBQ] to range between 1.10 or .90. These will occur at the beginning of simulation and should quickly approach 1.0 with additional time steps.

Figure 3-5. Comparison of maximum grid block δp results from the direct solver algorithm in the DWDM. The small graph shows the magnitude of relative difference between δp values.

Figure 3-6. Comparison of the solver output of maximum change in temperature (δT) between IBM and CDC results. The small graph shows the relative differences between the IBM and CDC results.

Figure 3-7. Heat loss calculation differences for IBM and CDC in an identical problem. The heat loss calculations by CDC (circles) are higher than by IBM (squares).

Figure 3-8. Fluid efflux across the outer boundary comparisons

Figure 3-9. Comparison of energy efflux at the periphery boundary

MISCELLANEOUS CHANGES

Most of the changes listed in this section have little or no effect on most final results. A number of these corrections are necessary when calling a certain group of options, for without these corrections, the code will fail. A number of modifications involved insertion of a checking statement to bypass a set of calculations that are unnecessary for a particular mode, and a number of other modifications check for divide check errors (division by zero) and underflow.

Some of the more important corrections and changes are listed as follows:

1. Overburden and underburden temperature are updated immediately after a time step, and options allow for printing of overburden and underburden temperature.
2. Manual entry of grid block size is allowed in radial coordinate mode.
3. Regional temperature modification is allowed in the aquifer as an initial condition in addition to temperature as function of depth.
4. Two dimensional x-z printer plotter maps are allowed.
5. Vertical radial coordinate flow transmissibility is changed to make calculations compatible with harmonic mean weighting used in cartesian coordinates.
6. Previous initial temperatures were assigned incorrect depths when calculating the initial geothermal profile in both reservoir and underburden and overburden. Corrections were applied so initial temperatures are assigned correct depth corresponding to the top grid block center in the reservoir. Similar corrections were applied to overburden and underburden blocks.
7. Dispersion tensor calculations were incorrect. The old equations used were

$$D_{xx} \tilde{u} = \tilde{u} [(\alpha_l \cos^2 \psi \cos^2 \theta) + \alpha_t (\sin^2 \theta + \sin^2 \psi \cos^2 \theta)]$$

$$D_{yy} \tilde{u} = \tilde{u} [(\alpha_l \cos^2 \psi \sin^2 \theta) + \alpha_t (\cos^2 \theta + \sin^2 \psi \sin^2 \theta)] .$$

The corrected equations are

$$D_{xx} \tilde{u} = \tilde{u}[(\alpha_l \cos^2 \psi \cos^2 \theta) + \alpha_t (\sin^2 \psi + \sin^2 \theta \cos^2 \psi)]$$

$$D_{yy} \tilde{u} = \tilde{u}[(\alpha_l \cos^2 \psi \sin^2 \theta) + \alpha_t (\sin^2 \psi + \cos^2 \theta \cos^2 \psi)]$$

where the latter set are found in equation (2-10).

8. All transmission coefficient output tables have dimensions associated with a printout option. Darcy velocity is calculated and printed as an option.
9. Overburden and underburden heat loss due to $\delta(T)$ had incorrect outer boundary conditions. The outer boundary condition was undefined. Correction was made by defining the outer boundary condition as zero.
10. The mapping routine uses variables that have the same names as those used in the iterative two-line successive overrelaxation routines. If a map is required, and solution is by two-line successive overrelaxation, the code will fail. Correction was made by changing variable names in the iterative solver.
11. A new option allowing manual core allocation entry for reordered Gaussian elimination solver was added. The code normally estimates the size of the [A] or [G(IAA)] array in the MAIN program. This is the working array in [SUBROUTINE GAUS3D]. The size allocated in the MAIN program must be larger than the quantity calculated in [SUBROUTINE ORDER]. If the core size allocated by the MAIN program is smaller than the amount needed as calculated by [ORDER], the core size for the [A] array in [GAUS3D] should be entered manually.

A few of the above changes were adapted from versions two and three of the code. All additional input option commands were designed in such a way that old input data require no modification in order to operate the simulator.

Underflow errors that originate in the solvers were left intact. These errors occur occasionally, are dependent upon problem parameters, and are handled by "FORTRAN Standard Fix-Up" which leaves a zero in the affected register. Experience has shown that these errors do not contribute to final results.

PART 4

SOLUTION COMPARISONS

PART 4

SOLUTION COMPARISONS

INTRODUCTION

This section consists of a number of solution comparisons of INTERCOMP and solutions derived by other means, either numerical or analytical. Comparisons are based on similar physical input data. Emphasis is given to test problems dealing with the energy equation.

Most test solutions used assume constant fluid density (ρ_w) and viscosity. In all of the problems, except where noted, changes in viscosity were kept at zero by defining constant viscosity in the viscosity tables. The density was allowed to vary; however, pressure and temperature were kept very close to base pressure and temperature (see equation 2-12) to minimize changes in density in the simulator. The a_3 term in equation (2-12) was zero to eliminate changes in density as a function of concentration. Likewise, a_2 was made small if free convection was noted in preliminary runs. In problems where only temperature and solute concentration are considered, pressure boundary input parameters are arbitrary except for one constraint. These parameters were designed to keep only the pressure in the aquifer near the base pressure (p_0).

A number of the solution comparisons are found in the INTERCOMP document (1976). A few of these solutions were run using different input param-

ters from those used in the INTERCOMP code verification. Most input data were kept as "real" as possible to check for the possibility of truncation errors.

The results displayed in this section are the code output after trying a number of mesh and time step sizes. This procedure was used to eliminate the possibility of solution dependence on mesh and time step magnitude.

THEIS SOLUTION

The flow equation and its corresponding mass balance was not a serious problem when compared to energy balance for the energy equation. However, for the sake of thoroughness, a check on fluid mass transport results from the DWDM was compared to the Theis solution (Theis, 1935, and Davis and DeWiest, 1966, p. 214). This problem simulates a single line source and unsteady fluid flow in a homogeneous isotropic confined aquifer of radially infinite extent. It is best described by

$$\frac{\partial^2 p}{\partial r^2} + \frac{1}{r} \frac{\partial p}{\partial r} = \frac{\mu(c_R + \phi c_w)}{k} \frac{\partial p}{\partial t} \quad (4-1)$$

with initial conditions

$$p(r, 0) = p_0$$

and boundary conditions

$$\lim_{r \rightarrow \infty} p = p_0 \quad \text{for } t > 0$$

$$\lim_{r \rightarrow 0} \left(r \frac{\partial p}{\partial r} \right) = \frac{Q\mu}{2\pi kb} \quad \text{for } t > 0$$

where b represents the total thickness of the reservoir and Q is the volumetric flow rate ($d(L^3t^{-1})$). The solution is

$$p = p_0 - \frac{Q\mu}{4\pi kb} \int_y^\infty \frac{e^{-x}}{x} dx \quad (4-2)$$

where

$$y = \frac{r^2(c_R + \phi c_w)\mu}{4kt}$$

The data for this problem are given in Table 4-1, and solution comparisons are given in Figure 4-1. The pressure variation shown in Figure 4-1 is based on an observation point 16.25 meters (53.3 feet) away from the line source, and the solution is based on an injection schedule of 25 days at 566.3 m^3 /day (2.00×10^4 ft^3 /day) followed by 0.0 m^3 /day for 25 days. In Figure 4-1, dimensionless pressure is defined as $(P - P_{min})/(P_{max} - P_{min})$, where P_{max} is 1.55×10^6 N/m^2 (225 psi) and P_{min} is 1.48×10^6 N/m^2 (215 psi), and dimensionless time = 1.0 is 50 days. The analytical solution based on the expansion of equation (4-2) is written as follows:

$$p = p_0 - \frac{Q\mu}{4\pi kb} [-.5772 - \ln(y) + y - \frac{y^2}{2 \cdot 2!} + \frac{y^3}{3 \cdot 3!} - \dots] \quad (4-3)$$

where y is defined in equation (4-2). The analytical solution after 25 days was obtained by superpositional techniques described in Davis and De Weist (1966). In summary, solution after 25 days is a summation of a solution involving injection, (negative Q) with time beginning at zero, and a solution involving production, (positive Q) which begins at time = 25 days.

Figure 4-1. Theis analytical solution comparison.

Table 4-1. Physical Data for Theis Solution Comparison

$c_R = 5.80 \times 10^{-10} \text{ l/N/m}^2$	(.000004 l/lbf/in ²)
$c_w = 4.35 \times 10^{-10} \text{ l/N/m}^2$	(.000003 l/lbf/in ²)
$\mu = 1.16 \times 10^{-8} \text{ N-day/m}^2$	(1.00 cp)
$K_x = K_z = k_{pg}/\mu g_c = 2.04 \text{ m/day}$	(6.68 ft/day)
$\phi = .18$	
$b = 61.0\text{m}$	(200 ft)
$\rho = 999.6 \text{ kg/m}^3$	(62.4 lbm/ft ³)
$Q = 566.3 \text{ m}^3/\text{day}$	(20000. ft ³ /day)
$r_e = 1524\text{m}$	(5000.0 ft)

SHAPE TEST PROBLEM

This exercise is designed to test the aquifer modification facility and zero pore volume flag of the INTERCOMP code. The zero pore volume flag is a means of by-passing blocks that have zero pore volume in the finite difference reservoir calculations in the INTERCOMP code.

The basic equation solved is

$$\frac{K_x}{\rho g} \frac{\partial^2 \psi}{\partial x^2} + \frac{K_y}{\rho g} \frac{\partial^2 \psi}{\partial y^2} = 0 \quad (4-4)$$

where

$$K = \text{hydraulic conductivity} = \frac{k_{pg}}{g_c \mu} \quad \text{and}$$

$$\psi = (\bar{v}p - \frac{\rho g}{g_c} \nabla z).$$

Since the INTERCOMP code is transient, the code was allowed to run until δp equals 0 for a given pair of source strengths. The actual flow domain used is given in Figure 4-2. Because the reservoir is "closed," the source strength calculations have to be exact; otherwise, pressure decline or increase is expected with time. Best results were obtained by using an explicit source where fluid flow is allocated by mobilities only.

The above was compared to a finite element solution of equation (4-4). Since the problem solved is steady state, the boundary conditions require a pressure and a source strength specification in the finite element formulation. Pressure was specified at the lower left-hand side of the flow field, and source strength was specified on the lower half of the right side of the flow field.

The Galerkin weighted function method was used to formulate the finite element problem. The Galerkin method requires

$$\int_D \nabla \cdot \frac{K}{\rho g} \nabla \psi N_i dD = 0 \quad (4-5)$$

where N_i is a suitable interpolation function defined by

$$\psi^{(e)} = [N^{(e)}] \{\psi\}^{(e)}$$

in which $\{\psi\}^e$ are nodal values. For this problem, 8-node quadratic elements of the serendipity family are used. Each reservoir element is mapped on a standard parent element by

$$\xi = \frac{x - x_c}{\frac{a}{2}} = \pm 1 \text{ or } 0$$

$$\eta = \frac{y - y_c}{\frac{b}{2}} = \pm 1 \text{ or } 0 \quad (4-6)$$

where a and b are horizontal and vertical element dimensions, and x_c and y_c are coordinates of the center of the element (see Figure 4-3). The solution is obtained by expanding equation (4-5), applying the Gauss theorem, and substituting equation (4-6) transformations to obtain the form

$$[k^*]\{\psi\}^{(e)} = \{r\}^{(e)} \quad (4-7)$$

where

$$k_{ij}^* = \frac{b}{a} \frac{K_x}{\rho g} \int_{-1}^1 \int_{-1}^1 \left\{ \frac{\partial N_i}{\partial \xi} \frac{\partial N_j}{\partial \xi} \right\} d\xi d\eta + \frac{a}{b} \frac{K_y}{\rho g} \int_{-1}^1 \int_{-1}^1 \left\{ \frac{\partial N_i}{\partial \eta} \frac{\partial N_j}{\partial \eta} \right\} d\xi d\eta$$

and

$$r_i = \frac{a}{2} \int_{-1}^1 (N_i - q_x) d\eta + \frac{b}{2} \int_{-1}^1 (N_i - q_y) d\xi.$$

The q_x and q_y are specific discharges at the flux boundary condition, and the interpolation functions used are

$$N_i = \frac{1}{2}(1 - \xi^2)(1 + \eta\eta_i), \quad \xi = 0, \quad \eta = \pm 1, \quad \text{nodes 2 and 6}$$

$$N_i = \frac{1}{2}(1 - \eta^2)(1 + \xi\xi_i), \quad \xi = \pm 1, \quad \eta = 0, \quad \text{nodes 8 and 4}$$

and

$$N_i = \frac{1}{2}(1 + \xi\xi_i)(1 + \eta\eta_i)(\xi\xi_i - \eta\eta_i - 1), \quad \xi = \pm 1, \quad \eta = \pm 1, \quad \text{corner nodes}$$

Figure 4-2. Reservoir schematic for shape test problem. Reduced permeability region is shown shaded.

Figure 4-3. Element to parent element relationship and numbering scheme.

where ξ_i and η_i refer to node values. Equation (4-7) for each element is combined to form a global equation of similar form for the domain. This equation was solved by the IBM scientific program package subroutine for a banded matrix GELB (IBM, 1970). The solution method used is similar to one found in p. 170-171 and p. 246-252 in Huebner, (1975). The physical data used are given in Table 4-2.

Since the actual equations and boundary conditions of the two compared problems differed, results are compared by relative pressure defined by

$$p_d = \frac{P - p_{\min}}{p_{\max} - p_{\min}}$$

where $p_{\max}$ = maximum pressure and $p_{\min}$ = minimum pressure in the reservoir, respectively. For isotropic flow domains, the results compared well (Figure 4-4); however, discrepancies appear near the source and sink in anisotropic flow domains (Figure 4-5).

The differences noted are partly attributed to differences in source location and slight domain differences. The INTERCOMP source is located half a block to the left and right of the inlet and outlet, respectively, and the means of allocation is by mobilities. The finite element uses flux strength at outlet and specified pressure at inlet for boundary conditions.

FINITE - DIFFERENCE PRESSURE

$$k_x = k_z$$

FINITE-ELEMENT PRESSURE

$$k_x = k_z$$

Figure 4-4. Dimensionless pressure distribution comparisons for an isotropic flow field.

Figure 4-5. Dimensionless pressure distribution comparisons for an anisotropic flow field.

Table 4-2. Physical Data for Shape Test

Fluid Density $\rho_w = 999.6 \text{ kg/ft}^3$	(62.4 lbm/ft ³)
Hydraulic Conductivity for $K_x = K_z = 859.5 \text{ m/day}$	(2820 ft/day)
Y-direction thickness = .305m	(1.0 feet)
Source Strength (Q) = 48.9 m ³ /day	(1728 ft ³ /day)
$\mu = 1.16 \times 10^{-8} \text{ N-day/m}^2$	(1.0 cp)
$\phi = .20$	

HOOPEES AND HARLEMAN PROBLEM

An approximate solution for the dispersion-diffusion equation in radial coordinates is given by Hoopes and Harleman (1967). This solution is used as an approximate verification of the code. For axisymmetric flow, the solute transport as given by Hoopes and Harleman is

$$\frac{\partial C}{\partial t} + q_r \frac{\partial C}{\partial r} = \alpha_L q_r \frac{\partial^2 C}{\partial r^2} + \frac{D_m}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) \quad (4-8)$$

where the hydrodynamic dispersivity factor is α_L , source flow rate is Q at $r = 0$, and velocities are defined as

$$q_r = \frac{Q}{2\pi b r \phi} = \frac{q}{\phi}$$

The Hoopes and Harleman solution assumes that at some distance away from the centralized line source the immediate effect of dispersion and diffusion on concentration is small in comparison to total dispersion and diffusion that

has already taken place. This approximation is applied to the right side of equation (4-8) by the substitution of

$$\frac{\partial(\cdot)}{\partial r} \approx -\frac{1}{q_r} \frac{\partial(\cdot)}{\partial t}$$

which, when used twice on equation (4-8) gives the result

$$\frac{\partial C}{\partial t} + q_r \frac{\partial C}{\partial r} = [\alpha_l \frac{1}{q_r} + D_m' \frac{1}{q_r^2}] \frac{\partial^2 C}{\partial t^2}. \quad (4-9)$$

The solution for equation (4-9) when a substance is injected at a steady rate at $r=0$ and a concentration of C_i is

$$\frac{C}{C_i} = \frac{1}{2} \operatorname{erfc} \left[\frac{\left(\frac{r^2}{2} - q_r t \right)}{\left(\frac{4}{3} \alpha_l r^3 + \frac{D_m'}{q_r} r^3 \right)^{1/2}} \right]. \quad (4-10)$$

This solution is an approximation to equation (4-8) with initial and boundary conditions

$$\begin{array}{llll} \text{at} & t = 0 & r \geq 0 & C = 0.0, \\ \text{at} & t > 0 & r = 0 & C_i = 1.0, \\ \text{and at} & t > 0 & \lim_{r \rightarrow \infty} & C = 0.0. \end{array}$$

Equation (4-8) is like the INTERCOMP solute equation in radial coordinates with the following basic assumptions:

1. Fluid density and porosity are constant and equal to $\rho\phi$, and
2. The dispersive flux coefficients $(\alpha_l q_r)$ and diffusion coefficients $(D_m' = D_m/\phi)$ are constants.

In the INTERCOMP code, the former assumption in (2) is not satisfied.

For heat transfer, the energy equation (2-6) written in the form of equation (4-8) is

$$\frac{\partial u}{\partial t} + q \frac{(\rho C_p)_w}{S} \frac{\partial u}{\partial r} = \left(\frac{(\rho C_p)_w}{S} \alpha_l q \right) \frac{\partial^2 u}{\partial r^2} + \frac{K_m}{rS} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right). \quad (4-11)$$

where

S = heat capacity of matrix plus water, or

$$(\phi(\rho C_p)_w + (1 - \phi)(\rho C_p)_R)$$

and

$$u = \frac{T - T_0}{T_i - T_0} \text{ for dimensionless temperature.}$$

Equation (4-10) is an approximate solution to equation (4-11) with the following initial and boundary conditions:

$$\begin{array}{llll} \text{at} & t = 0 & r \geq 0 & u = 0.0, \\ & & & \\ & \text{at} & t > 0 & r = 0 \quad u = 1.0, \\ & & & \\ \text{and at} & t > 0 & \lim_{r \rightarrow \infty} & u = 0.0. \end{array}$$

The results of this analysis are given in Figures 4-6 and 4-7. In Figure 4-6, maximum dimensionless radius is 30.48m (100 ft), maximum dimensionless temperature (u) is equal to 37.78° C (100° F), and minimum u is equal to 21.11° C (70° F). In Figure 4-7, maximum dimensionless radius is 60.96m (200 ft). The physical data are given in Table 4-3.

The results from the INTERCOMP test problem tend to lag behind the analytical results from equation (4-10) with the greatest deviations at dimensionless units of 0.00 and 1.00. This characteristic pattern is also seen in the paper by Hoopes and Harleman who show better solution matches as time proceeds. Part of the difference comes from the fact that equation (4-10) predicts a finite quantity of substance at $t=0$, unlike no substance specified by

the original initial condition. This error comes from substituting a first-order space derivative with the time derivative where

$$\frac{\partial(\cdot)}{\partial t} = \left(-\frac{1}{q_r}\right) \frac{\partial(\cdot)}{\partial t} = 0$$

at $t=0$. This assumption is not true at early time near the source (Hoopes and Harleman, 1967).

Figure 4-6. Hoopes and Harleman solution comparison.

Figure 4-7. Solute concentration comparison to Hoopes and Harleman analytical solution.

Table 4-3. Physical Data for Hoopes and Harleman Solution

$\alpha_l = .30\text{m}$	(1.0 ft)
$D_m = .11 \text{ m}^2/\text{day}$	(1.16 ft ² /day)
$(\rho C_p)_R = 2.01 \times 10^6 \text{ J}/(\text{m}^3 \text{ }^\circ\text{K})$	(30 Btu/(ft ³ °F))
$(C_p)_w = 4.19 \times 10^3 \text{ J}/(\text{kg } ^\circ\text{K})$	(1.0 Btu/(lbm °F))
$K_m = 8.37 \text{ W}/(\text{m } ^\circ\text{K})$	(116. Btu/(ft-day °F))
$Q = 49.70 \text{ m}^3/\text{day}$	(1755 ft ³ /day)
$\rho_w = 1.00 \times 10^3 \text{ kg}/\text{m}^3$	(62.4 lbm/ft ³)
$\phi = .10$	
$\mu = 2.31 \times 10^{-8} \text{ N-day}/\text{m}^2$	(2.0 cp)
$k_x \rho g / g_c \mu = 120.1 \text{ m}/\text{day}$ (hydraulic conductivity)	(394. ft/day)
$T_o = 21.11 \text{ }^\circ\text{C}$	(70 °F)
$T_i = 37.78 \text{ }^\circ\text{C}$	(100 °F)
$b = 9.14 \text{ m}$	(30.0 ft)
$r_e = 91.44 \text{ m}$ (external radius)	(300 ft)

ONE DIMENSION TEST

The linear one-dimensional DWDM solution is compared to a solution given by Brenner (1962) and Coats and Smith (1964). The equation solved in these papers is

$$E_C^* \frac{\partial^2 C}{\partial x^2} - q_r \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (4-12)$$

where

$$E_C^* = \frac{E_C}{\phi}$$

with initial and boundary conditions

$$0 \leq x \leq \infty$$

$$C(x, 0) = 0.0$$

$$x = 0.0 \quad (t > 0)$$

$$qC_i = qC - E_C \frac{\partial C}{\partial x} \quad (C_i = 1.0)$$

$$x \rightarrow \infty \quad (t > 0)$$

$$C(x, t) = 0.0$$

where q_r = average pore velocity. The solution is

$$\begin{aligned} \frac{C}{C_i} = & \frac{1}{2} \left[\operatorname{erfc} \left(\frac{\sqrt{Y}}{2} \frac{Y - I}{\sqrt{I}} \right) - e^{YI} \operatorname{erfc} \left(\frac{\sqrt{Y}}{2} \frac{Y + I}{\sqrt{I}} \right) \right] \\ & - \frac{Y}{2} (Y + I) e^{YI} \operatorname{erfc} \left(\frac{\sqrt{Y}}{2} \frac{Y + 1}{\sqrt{I}} \right) + \sqrt{\frac{YI}{\pi}} e^{\left(-\frac{Y}{4I} (Y - I)^2 \right)}. \end{aligned} \quad (4-13)$$

Assuming constant dispersive flux, density, porosity and thermal properties, the DWDM equations in one dimension can be written as

$$\frac{E_C}{\phi} \frac{\partial^2 C}{\partial x^2} - q_r \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (4-14)$$

and

$$\frac{E_H}{S} \frac{\partial^2 T}{\partial x^2} - \frac{\phi (\rho C_p)_w q_r}{S} \frac{\partial T}{\partial x} = \frac{\partial T}{\partial t} \quad (4-15)$$

where

$$q_r = \frac{q}{\phi}$$

$$\frac{E_C}{\phi} = \alpha_l q_r + \frac{D_m}{\phi}$$

$$\frac{E_H}{S} = \frac{\phi (\rho C_p)_w \alpha_l q_r + K_m}{S}$$

and

$$S = (\phi(\rho C_p)_w + (1 - \phi)(\rho C_p)_R).$$

The parameters for equation (4-13) are

$$\gamma = \frac{q_r \phi L}{(\alpha_\ell q_r \phi + D_m)}$$

$$y = \frac{x}{L}$$

$$I = \frac{q_r t}{L}$$

and

$$\gamma = \frac{q_r \phi (\rho C_p)_w L}{(\alpha_\ell q_r \phi (\rho C_p)_w + K_m)}$$

$$y = \frac{x}{L}$$

$$I = \frac{q_r \phi (\rho C_p)_w t}{SL}$$

for the solute (4-14), and energy (4-15) equations, respectively. Comparison results are shown in Figures 4-8 and 4-9, and physical data are listed in Table 4-4. Analytical results compare very well with the INTERCOMP numerical results. This is expected because equation (4-12) can be derived directly from simplification of the INTERCOMP generalized equations. The use of constant total dispersivity fits well with a one dimensional linear problem because q remains constant throughout the solution domain; hence, E_c is a constant.

Table 4-4. Physical Data for One-dimensional Linear Solution

$(\rho C_p)_R = 2.01 \times 10^6 \text{ J/m}^3 \text{ } ^\circ\text{K}$	(30.00 Btu/ft ³ °F)
$(C_p)_w = 4.19 \times 10^3 \text{ J/kg } ^\circ\text{K}$	(1.0 Btu/lbm °F)
$\rho_w = 1.00 \times 10^3 \text{ kg/m}^3$	(62.40 lbm/ft ³)
$K_m = 2.16 \text{ W/m } ^\circ\text{K}$	(30.00 Btu/ft day °F)
$Q = 2.83 \times 10^{-3} \text{ m}^3/\text{day}$	(.10 ft ³ /day)
$b = .30 \text{ m}$	(1.00 ft)
$\mu = 1.16 \times 10^{-8} \text{ N-day/m}^2$	(1.00 cp)
$T_o = 21.11 \text{ } ^\circ\text{C}$	(70.00 °F)
$T_i = 37.78 \text{ } ^\circ\text{C}$	(100.00 °F)
hydraulic conductivity = $k_{pg}/g_c\mu = 61.0 \text{ m/day}$	(200. ft/day)
$D_m = 0.0 \text{ m}^2/\text{day}$	
$\alpha_l = 15.85 \text{ m}$	(52.00 ft)

Figure 4-8. One-dimensional temperature solution comparisons. Length equal to 1.0 is the same as 198.12m (650 ft).

Figure 4-9. Solute concentration solution comparisons. Length equal to 1.0 corresponds to 381.00m (1250 ft).

AVDONIN PROBLEM

In a realistic heat storage problem, the confining overburden and underburden rocks conduct thermal energy away from the aquifer. The DWDM estimates this heat loss by simulating one-dimensional transient heat conduction in the overlying and underlying rocks. Avdonin (1964) presented an analytical solution to heat transfer in the aquifer by convection and heat loss by conduction in radial and one-dimensional flow patterns. His problem is best described by the dimensionless equation for the aquifer (storage reservoir)

$$\frac{\partial^2 u}{\partial r_d^2} + \frac{(1 - 2\nu)}{r_d} \frac{\partial u}{\partial r_d} + \alpha \left. \frac{\partial u}{\partial z_d} \right|_{z_d=0} = \frac{\partial u}{\partial t_d} \quad (4-16)$$

where $z_d = 0$ signifies aquifer base depth, and subscript d indicates a dimensionless variable. The initial and boundary conditions for equation (4-16) are

$$\begin{array}{lll} t_d = 0 & u = 0.0 & \text{for all } r_d \text{ and } z_d \\ t_d > 0 & u = 1.0 & \text{for } r_d = z_d = 0 \\ t_d > 0 & u = 0.0 & \text{for } r_d + z_d = \infty \end{array}$$

Heat transfer in the overburden and underburden is represented by the dimensionless equation

$$\frac{\partial^2 u}{\partial z_d^2} = a \frac{\partial u}{\partial t_d} \quad (4-17)$$

The undefined coefficients in equations (4-16) and (4-17) are

$$\nu = \frac{Q(\rho C_p)_w}{4\pi b K_m}$$

$$\alpha = \frac{K_{ob}}{K_m}$$

and

$$a = \frac{(\rho C_p)_{ob} K_m}{K_{ob} (\rho C_p)_m}$$

and dimensionless variables defined by subscript d are

$$r_d = \frac{2r}{b}$$

$$z_d = \frac{2z}{b}$$

and

$$t_d = \frac{4}{b^2} \frac{K_m}{(\rho C_p)_m} t.$$

The solution to this problem is given as

$$u(r_d, t_d) = \frac{1}{\Gamma(\nu)} \left(\frac{r_d^2}{4t_d} \right)^\nu \int_0^1 \left(\exp \left(-\frac{r_d^2}{4t_d x} \right) \cdot \operatorname{erfc} \left(\frac{\alpha \sqrt{a} \sqrt{t_d} x}{\sqrt{1-x}} \right) \frac{1}{x^{\nu+1}} \right) dx \quad (4-18)$$

Equations (4-16) and (4-17) can be derived directly from the DWDM radial flow equations after dropping the total dispersivity term. The following are used to substitute for space, time, and temperature variables:

$$r = \frac{r_d b}{2}$$

$$z = \frac{z_d b}{2}$$

$$t = \frac{(\rho C_p)_m b^2}{K_m} \frac{1}{4} t_d$$

and

$$u = \frac{T - T_0}{T_i - T_0}$$

where

$$(\rho C_p)_m = (\phi (\rho C_p)_w + (1 - \phi) (\rho C_p)_R).$$

The DWDM solution used a 20 x 1 x 2 node mesh to simulate the above problem. This selection was chosen in order to use both direct solution (Price and Coats, 1964) and two-line successive overrelaxation solvers. The results obtained from both solvers were identical and are given in Figure 4-10. The effect of free convection was sufficiently small, so results compared well with the analytical one-dimensional radial flow solution by Avdonin.

A second comparison in Figure 4-11 shows the result of DWDM using a linear 20 x 20 x 1 grid with the well located at node 1, 1, 1 (lower left corner), and simulation results are measured in the upper right-hand quadrant of an infinite circular aquifer. The physical data for this problem are listed in Table 4-5.

Avdonin also solved the linear one dimensional version of equation (4-16). The resultant dimensionless aquifer equation becomes

$$\frac{\partial^2 u}{\partial x_d^2} - 2\gamma \frac{\partial u}{\partial x_d} + \alpha \frac{\partial u}{\partial z_d} \bigg|_{z_d=0} = \frac{\partial u}{\partial t_d} \quad (4-19)$$

where

$$\gamma = \frac{Q^* (\rho C_p)_w}{4K_m} \quad (1), \quad Q^* = qb, \quad d(L^2 t^{-1})$$

and

$$x_d = \frac{2x}{b}.$$

This equation, as explained earlier, is the same as the linear energy equation used by INTERCOMP after it was made dimensionless by proper substitutions.

The transient heat loss by conduction is the same as equation (4-17), and initial and boundary conditions are

$$\begin{aligned} t_d = 0 & \quad u = 0.0 & \quad \text{for all } x_d \text{ and } z_d \\ t_d > 0 & \quad u = 1.0 & \quad \text{for } x_d = z_d = 0 \\ t_d > 0 & \quad u = 0.0 & \quad \text{for } x_d + z_d = \infty. \end{aligned}$$

The solution given by Avdonin is

$$\begin{aligned} u(x_d, t_d) = & \frac{x_d}{\sqrt{\pi t_d}} \int_0^1 \left\{ \exp \left[- (sy\sqrt{t_d} - \frac{x}{2s\sqrt{t_d}})^2 \right] \right. \\ & \left. \cdot \operatorname{erfc} \left[\frac{\alpha\sqrt{a}\sqrt{t}}{2} \frac{s^2}{\sqrt{1-s^2}} \right] \frac{1}{s^2} \right\} ds. \end{aligned} \quad (4-20)$$

The comparisons of the linear one-dimensional solution are given in Figures 4-12 and 4-13. The differences in Figure 4-12 are partly due to disparities in boundary conditions at the source, the finite thickness of the overburden and numerical diffusion. Approximate calculations presented in Karlekar and Desmond (1977, p. 133-139) show that the conduction thermal front

¹ The corrected formula is given by Faust and Mercer (1979).

reaches the outer overburden node at $z = 10.97\text{m}$ (36 ft) where temperature is held at $T = T_0$; hence, the expected thermal conduction gradient is slightly greater in the DWDM than in the Avdonin solution with $T = T_0$ at $z = \infty$.

This was also verified by overburden temperature print-out. Since the problem was run using Crank-Nicholson and upwind in space the numerical diffusion defined by $u\Delta x/2$, for upwind differencing, gets larger at the outerblocks because Δx is larger, while u (Darcy velocity) remains constant. This is unlike radial coordinate problems because u decreases by a factor of $1/r$. Better comparisons are obtained when the thickness of the overburden is increased to $z = 18.29\text{m}$ (60 ft), and the number of finite difference reservoir blocks are increased (Figure 4-13).

Figure 4-10. Radial Avdonin problem comparisons. Maximum dimensionless radius corresponds to 15.24m (50 ft).

Figure 4-11. Radial Avdonin problem compared to a cartesian coordinate approximation solution. Maximum radius of 1.0 corresponds to 15.25m (50 ft).

Figure 4-12. One-dimension linear Avdonin solution comparison results.
Dimensionless length of 1.0 corresponds to 30.48m (100 ft).

Figure 4-13. One-dimension linear Avdonin solution comparison results with extended overburden boundaries and higher node density. Dimensionless length of 1.0 corresponds to 30.48m (100 ft).

Table 4-5. Physical Data for Avdonin Solution

Data for Radial Solution:

$(\rho C_p)_R = 2.84 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	(42.45 Btu/(ft ³ °F))
$(C_p)_w = 4.19 \times 10^3 \text{ J/(kg }^\circ\text{K)}$	(1.00 Btu/(lbm °F))
$(\rho C_p)_{ob} = 2.43 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	(36.3 Btu/(ft ³ °F))
$\rho_w = 1.00 \times 10^3 \text{ kg/m}^3$	(62.4 lbm/ft ³)
$K_m = K_{ob} = 2.42 \text{ W/(m }^\circ\text{K)}$	(33.6 Btu/(ft-day °F))
$Q_w = 3.78 \text{ m}^3/\text{day}$	(133.60 ft ³ /day)
$b = 3.05\text{m}$	(10.00 ft)
$\phi = .20$	
$\mu = 1.16 \times 10^{-8} \text{ (N-day)/m}^2$	(1.00 cp)
$T_o = 21.11 \text{ }^\circ\text{C}$	(70.00 °F)
$T_i = 37.78 \text{ }^\circ\text{C}$	(100.00 °F)
hydraulic conductivity = $k_{pg}/\mu g_c = 60.96 \text{ m/day}$	(200.00 ft/day)

Data for Linear Solution:

$(\rho C_p)_R = 2.01 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	(30.00 Btu/(ft ³ °F))
$(C_p)_w = 4.19 \times 10^3 \text{ (J/kg }^\circ\text{K)}$	(1.00 Btu/(lbm °F))
$(\rho C_p)_{ob} = 2.01 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	(30.00 Btu/(ft ³ °F))
$\rho_w = 1.00 \times 10^3 \text{ kg/m}^3$	(62.4 lbm/ft ³)
$K_m = K_{ob} = 2.16 \text{ W/(m }^\circ\text{K)}$	(30.00 Btu/(ft-day °F))
$Q_w = 1.13 \text{ m}^3/\text{day}$	(40.00 ft ³ /day)
$b = 3.05\text{m}$	(10.00 ft)
$\phi = .10$	
$\mu = 1.16 \times 10^{-8} \text{ (N-day)/m}^2$	(1.00 cp)
$T_o = 21.11 \text{ }^\circ\text{C}$	(70.00 °F)
$T_i = 37.38 \text{ }^\circ\text{C}$	(100.00 °F)
hydraulic conductivity = $k_{pg}/\mu g_c = 60.96 \text{ m/day}$	(200.00 ft/day)

GRINGARTEN AND SAUTY SOLUTION

This problem consists of an infinite uniform reservoir of thickness b , tapped by a fully penetrating source and sink of equal strength separated by a distance, d . The overburden and underburden are infinite in the vertical direction. The initial temperature is T_0 , and injection temperature is T_i . Thermal conductivity is neglected in the aquifer (reservoir) in the horizontal direction (high Peclet number), and temperature is assumed uniform in the vertical direction in the aquifer. Heat conduction in the overburden and underburden take place only in the vertical direction, and all thermal and fluid properties are assumed constant. This problem is like the Avdonin problem except the domain contains a source and a sink.

The basic equation that satisfies the criteria expressed above for the aquifer operating along an infinitesimal stream channel $\psi + \Delta\psi$ (Figure 4-14) is

$$\begin{aligned} \frac{b}{2} (\rho C_p)_m \frac{\partial T}{\partial t} + \frac{q}{2} (\rho C_p)_w \frac{\partial T}{\partial A} &= K_{ob} \frac{\partial T_{ob}}{\partial z} \bigg|_{z=\frac{b}{2}} \quad (4-21) \\ \text{(Accumulation)} \quad \quad \quad \text{(Net Convection)} \quad \quad \quad \text{(Heat Loss via Overburden)} \end{aligned}$$

where

$$T = T^\psi(A, \frac{b}{2}, t)$$

$$T_{ob} = T_{ob}^\psi(A, z, t) \quad z \geq \frac{b}{2}$$

$$(\rho C_p)_m = (\phi (\rho C_p)_w + (1 - \phi) (\rho C_p)_R)$$

The variable A equals the cumulative surface area (dimensionless) between the source and point of interest in the flow field, $z = b/2$ designates the location of the overburden and underburden contact boundary, and q is the Darcy velocity.

The overburden temperature is governed by

$$\frac{\partial^2 T_{ob}}{\partial z^2} = \frac{(\rho C_p)_{ob}}{K_{ob}} \frac{\partial T_{ob}}{\partial t} \quad z \geq \frac{b}{2} \quad (4-22)$$

where the subscript ob designates overburden. Since the temperature in the aquifer is uniform in the vertical, total heat loss is twice the heat loss to the overburden. Equations (4-21) and (4-22) are bounded by the following conditions:

$$T_{ob} = T = T_0 \quad qt < \phi bA \text{ (ahead of hydrodynamic front)}$$

$$T(0, t) = T_0 \quad t \leq 0$$

$$T(0, t) = T_i \quad t > 0, \text{ and}$$

$$\lim_{z \rightarrow \infty} T = T_0.$$

The temperature distribution in a given stream channel adapted from the Lauwerier (1955) solution is

$$\frac{T_0 - T}{T_0 - T_i} = \operatorname{erfc} \left[\frac{(\rho C_p)_w^2}{K_{ob} (\rho C_p)_{ob}} \left(\frac{q}{A} \right)^2 \left(t - \frac{(\rho C_p)_m bA}{(\rho C_p)_w q} \right) \right]^{-1/2} \quad (4-23)$$

The temperature of the fluid at the production well--that is, at the end of the stream channel--is determined by substituting A for A_t = total "area" of

the stream channel. In most cases, A_t has to be determined numerically. Temperature in the production well at time t is therefore the summation of contributions from all the stream channels that have reached the production well at time t .

This solution has no nice closed form equation which gives the resultant temperature at the production well; hence, comparisons were made to Figure 6 in the paper by Gringarten and Sauty (1975). The results are given in Figure 4-15, and physical data are given in Table 4-6. The range of temperature used in this problem goes from a maximum of 26.67°C (80°F) to a minimum of 15.56°C (60°F). The last point response from the INTERCOMP code corresponds to 500 days. An areal map using the second set of data ($\lambda = 6.00$) is given in Figure 4-16.

The INTERCOMP code is simulated by assuming symmetry along the axis connecting the injection and production well using a $48 \times 18 \times 1$ grid for 500 days. The outer periphery is assumed as infinite, and is estimated by the Carter-Tracy aquifer influence functions. Figure 6 in Gringarten and Sauty's paper assumes $Q_D = Q/(bd u_o) > 10^4$ where d is the distance between injection and production wells, u_o is the natural between the sink and the source Darcy velocity, and Q is the total injection rate which is equal to the production rate. This condition is satisfied by setting $u_o = 0$ in the INTERCOMP input.

The dimensionless parameters for Figure 4-15, as defined by Gringarten and Sauty, are

$$\lambda = \frac{(\rho C_p)_w (\rho C_p)_m Q_D b}{K_{ob} (\rho C_p)_{ob} d^2}$$

$$u = \frac{T_0 - T(t)}{T_0 - T_i} \quad (\text{dimensionless temperature})$$

and

$$t_d = \frac{(\rho C_p)_w}{(\rho C_p)_m} \frac{Q t}{d^2 b}.$$

Figure 4-14. Nomenclature for an arbitrary stream channel. The variable A is a dimensionless area.

Figure 4-15. Comparison of the Gringarten and Sauty problem with INTERCOMP results. (Continuous results are adapted from Gringarten and Sauty, 1975, Figure 6.)

Figure 4-16. Areal map of temperature distribution at time = 500 days for $\lambda = 6.00$.

Table 4-6. Physical Data for Gringarten and Sauty Problem

$(\rho C_p)_R = 2.01 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	$(30.00 \text{ Btu/(ft}^3 \text{ }^\circ\text{F)})$
$(C_p)_w = 4.19 \times 10^3 \text{ J/(kg }^\circ\text{K)}$	$(1.00 \text{ Btu/(lbm }^\circ\text{F)})$
$\rho_w = 1.00 \times 10^3 \text{ kg/m}^3$	(62.4 lbm/ft^3)
$(\rho C_p)_{ob} = 2.01 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	$(30.00 \text{ Btu/(ft}^3 \text{ }^\circ\text{F)})$
$\phi = .20$	
$(\rho C_p)_m = 2.44 \times 10^6 \text{ kg/(m}^3 \text{ }^\circ\text{K)}$	$(36.48 \text{ Btu/(ft}^3 \text{ }^\circ\text{F)})$
$b = 1.00 \text{ m}$	(3.28 ft)
$d = 15.00 \text{ m}$	(49.21 ft)
$Q = 54.00 \text{ m}^3/\text{day}$	$(1906.80 \text{ ft}^3/\text{day})$
$K_{ob} = 2.35 \text{ W/(m }^\circ\text{K)}$	$(32.6 \text{ Btu/(ft-day }^\circ\text{F)})$

Graphical Parameters:

$$\lambda = 6.00$$

$$t_d = .410 t \quad \text{for } t \text{ in days.}$$

$(\rho C_p)_R = 2.01 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	$(30.00 \text{ Btu/(ft}^3 \text{ }^\circ\text{F)})$
$(C_p)_w = 4.19 \times 10^3 \text{ J/(kg }^\circ\text{K)}$	$(1.00 \text{ Btu/(lbm }^\circ\text{F)})$
$\rho_w = 1.00 \times 10^3 \text{ kg/m}^3$	(62.4 lbm/ft^3)
$(\rho C_p)_{ob} = 2.01 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	$(30.00 \text{ Btu/(ft}^3 \text{ }^\circ\text{F)})$
$\phi = .20$	
$(\rho C_p)_m = 2.44 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	$(36.48 \text{ Btu/(ft}^3 \text{ }^\circ\text{F)})$
$b = 10.00 \text{ m}$	(32.81 ft)
$d = 15.00 \text{ m}$	(49.21 ft)
$Q = 540 \text{ m}^3/\text{day}$	$(19068.0 \text{ ft}^3/\text{day})$
$K_{ob} = 8.36 \times 10^{-2} \text{ W/(m }^\circ\text{K)}$	$(1.16 \text{ Btu/(ft-day }^\circ\text{F)})$

Graphical Parameters:

$$\lambda = 1.68 \times 10^4$$

$$t_d = .410 t \quad \text{for } t \text{ in days.}$$

Listing of Nonessential Hydraulic Parameters

$$K_x = K_y = 244 \text{ ft/day}$$

(800 ft/day)

$$\mu = 1.16 \times 10^{-8} \text{ (N-day)/m}^2$$

(1.0 cp)

PART 5

AUBURN UNIVERSITY FIELD EXPERIMENT

PART 5

AUBURN UNIVERSITY FIELD EXPERIMENT

INTRODUCTION

This section compares simulated results with field experiment results from an ATES research project carried out by Auburn University near Mobile, Alabama. Results of the INTERCOMP simulation response are also compared to those derived from the Lawrence Berkeley Laboratory CCC code (Tsang, Buscheck, and Doughty, 1981).

The application described in this section requires solution of the energy and pressure equations using the nonlinear solution capabilities of the code. The reader should note that the solution used for this simulation is a gross approximation based on known data about the aquifer. For instance, a truly "correct" simulation should not be based on an axisymmetrical aquifer.

EXPERIMENT AND SIMULATION

The final test problem is a comparison between the DWDM and an on-going research program of the ATES concept sponsored by the DOE and administered by the Water Resources Research Institute of Auburn University. The project site is located near the Barry Steam Plant of the Alabama Power Company, about 32.2 km (20 miles) north of Mobile, Alabama (Moltz, Warman, and Jones, 1978).

Data used in this simulation are the result of several earlier studies and simulations. In 1976, Auburn University completed the first set of field experiments storing 35° C (95° F) treated (filtered and chlorinated) condenser cooling water obtained from a drainage canal of the power plant. Analysis of the data and a numerical simulation using the INTERCOMP code (version one) were performed by Papadopoulos and Larson (1978). Experimental problems caused by clogging of the storage aquifer and breaching the confining layer appear to be the primary causes of differences between the predicted (by simulation) recovery ratio of 0.75 and the observed recovery ratio of 0.69. Discussion about experimental problems are given in Moltz et al. (1978).

The series of experiments being simulated in this section were conducted between March 18, 1978, and January 27, 1979, and covered two injection, storage, and recovery cycles separated by 20 days. The first cycle consisted of injecting 54,800 m³ (1.94×10^6 ft³) of water at an average temperature of 55 °C for a period of 79 days, followed by a 50.5-day storage period and a production volume of 55,300 m³ (1.95×10^6 ft³) over a period of 41 days. The second cycle, begun on September 23, 1978, consisted of injecting 58,010 m³ (2.05×10^6 ft³) of water over a period of 64 days, followed by storage of 63 days, and further production of a volume of 100,100 m³ (3.53×10^6 ft³) over a period of 84 days. Technical problems with the latest series of experiments are discussed in Moltz, Parr, and Anderson (1980).

The basic experimental configuration is shown in Figures 5-1 and 5-2. The well field consists of a group of instrumented observation wells and an injection or production well tapping into an aquifer located between 39.6 m (130 ft) and 61 m (200 ft) beneath the surface. Unlike the first experiment, sediment-free ground water is obtained from a supply aquifer located between

25 m (82 ft) and 34 m (112 ft) beneath the surface. Twenty degree centigrade (68.00° F) water obtained from the supply aquifer is heated to about 55° C (131.00° F) and injected into the storage aquifer at injection well #2 through a well screen extending from a depth of 42.4 m (139 ft), to 51.5 m (169 ft).

The storage formation is composed of sand with 15% silt and clay by weight. The aquifer is capped by 9.0 m (30 ft) of impermeable clay and is bounded below by another impermeable formation of clay of undetermined thickness. The supply aquifer overlies the upper clay layer. The sequence of materials is part of a buried river channel which has one relatively long dimension.

Aquifer physical data were obtained from earlier research by Papadopoulos and Larson (1978). In this study, well pumping tests show transmissivity and storage coefficient to be 940 m²/day (10,000 ft²/day) and 5.0 x 10⁻⁴, respectively as obtained by Theis type curve analysis (Davis and DeWeist, 1966, p. 215). Also noted in this study were two departures from the Theis curve, which signify at least two hydraulic boundaries. Graphical methods using image wells (Ferris, Knowles, Browne and Stallman, 1962) failed to place these hydraulic boundaries; however, a more recent study at LBL using a code ANALYZE to study multiwell pressure data (Doughty, McEdwards, and Tsang, 1979) has placed hydraulic parameters as

$$\text{Transmissivity} = \frac{kb}{\mu} = .109 \times 10^7 - .118 \times 10^7 \frac{\text{md} - \text{m}}{\text{cp}}$$

(md = millidarcy unit)

$$\text{or, assuming } b = 21.3\text{m (70ft)}, \frac{\rho g}{g_c} = 62.3 \text{ lb/ft}^3$$

$$K = 3000\text{m/day (9800ft/day)} - 3230\text{m/day (10600ft/day)}$$

$$\text{Storativity} = \frac{\rho g}{g_c} b (c_R - \phi_{cw}) = .464 \times 10^{-3} - .484 \times 10^{-3}$$

with the nearest boundary at the northwest side of the well field at a distance between 305m (1000 ft) to 337m (1100 ft). The program ANALYZE uses transmissivity, storage coefficient, angle of boundary, and distance to boundary to compute pressures by assuming fully penetrating line sources or sinks in an aquifer of constant thickness. The program arrives at an optimum set of hydraulic parameters by a least squares minimization of computed pressures and observed pressures. Other general trends noted in this study were that hydraulic conductivity decreases from south to north and storativity and porosity decrease from southeast to northwest. Such trends are consistent with the general theory that the boundary at the northwest of the well field is one edge of a buried river channel.

Natural hydraulic gradients are suggestive of approximate natural Darcy flow velocity of .05 m/day (.17 ft/day) from northerly to southerly direction; hence, the expected fluid movement during a 70 day span is 3.5 m (11.5 ft) (Moltz, et al., 1980).

The best representative ratio of horizontal to vertical permeability (K_r/K_z) is 10. This ratio has been confirmed by simulation by Papadopoulos and Larson (1978) Moltz et al. (1978), and more recently by LBL (Tsang, Buscheck, and Doughty, 1980). Thermal properties were obtained from laboratory studies completed for the earlier simulation by Papadopoulos and Larson.

Like earlier work completed by Papadopoulos and Larson (1978) and simulation by LBL, it is impractical to simulate the experiments using three dimensions. This is because of lack of a precise hydraulic boundary and hydrologic data and high machine time costs. The choice of conceptual model is a homogeneous anisotropic confined aquifer of infinite extent in the horizontal direction with one-dimensional thermal conduction losses through the

confining layers. Since the expected movement of the thermal plume is about 0.05 m/day (0.17 ft/day), the conceptual model is best assumed to be axisymmetric about the injection-production well. In general, all physical data are taken to be the same as those used by Papadopoulos and Larson (1978) except that longitudinal hydrodynamic dispersivity is taken as zero instead of 5.0 ft (1.52 m).

Table 5-1 summarizes the input data used in simulating the Mobile experiment. The density tables compare model responses to actual measurements with pure water. The viscosity table is a listing of viscosities at various temperatures that are used as input for the model.

The chosen radial mesh size is given in Figure 5-3. The cross marks are locations of grid block centers for the reservoir, and horizontal lines in the overburden and underburden blocks designate input mesh rather than the actual mesh dimensions (see Appendix B). This is the finer of two mesh sizes used in the simulation. The grid block size in the region occupied by the thermal plume at its maximum extent is roughly the same density as the LBL medium mesh (Tsang, et al., 1981). Two-dimensional transient radial flow is assumed in the storage formation, and one-dimensional transient heat conduction is assumed in the overburden and underburden. An infinite aquifer influence function is attached to the outer periphery boundary.

The pumping and recovery cycle input data for cycles one and two are given in Figures 5-4, 5-5 and 5-6. These recurrent injection and production data are the same as those used in the CCC code simulation provided by LBL. In Figure 5-4, the heavy lines are data used for the simulation by LBL and INTERCOMP. Short increments of very high flows are truncated at 1500 m³/day (5.30×10^4 ft³/day) in order to provide for a reasonable graph ordinate.

Likewise in Figures 5-5 and 5-6, the heavy lines are data used for the simulation, provided by LBL.

Figure 5-1. Plan view of the Mobile ATES experiment well field. Injection well 2 is used for this experiment.

Figure 5-2. Sectional schematic of the Mobile experiment (adapted from Moltz et al., 1980).

Figure 5-3. Finite difference radial mesh for the Mobile experiment simulation.

Figure 5-4. Injection rate and temperature for first cycle simulation.

Figure 5-5. Injection rate and temperature for second cycle simulation.

Figure 5-6. Production rates for cycles one and two.

Table 5-1. Physical Data for the Mobile Experiment

Aquifer Properties:

$(\rho C_p)_R = 1.81 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	$(27.00 \text{ Btu/ft}^3 \text{ }^\circ\text{F)}$
$(C_p)_w = 4.19 \times 10^3 \text{ J/(kg }^\circ\text{K)}$	$(1.00 \text{ Btu/lbm }^\circ\text{F)}$
$(\rho C_p)_{ob} = 1.81 \times 10^6 \text{ J/(m}^3 \text{ }^\circ\text{K)}$	$(27.00 \text{ Btu/ft}^3 \text{ }^\circ\text{F)}$
$(\rho C_p)_{ub} = (\rho C_p)_{ob}$	
$K_m = 2.29 \text{ W/(m }^\circ\text{K)}$	$(31.80 \text{ Btu/ft-day }^\circ\text{F)}$
$K_{ob} = 2.56 \text{ W/(m }^\circ\text{K)}$	$(35.5 \text{ Btu/ft-day }^\circ\text{F)}$
$K_{ob} = K_{ub}$	
$c_w = 4.44 \times 10^{-10} \text{ 1/(10/m}^2\text{)}$	$(3.06 \times 10^{-6} \text{ 1/(lbf/in}^2\text{)})$
$c_R = 2.28 \times 10^{-9} \text{ 1/(N/m}^2\text{)}$	$(1.57 \times 10^{-5} \text{ 1/(lbf/in}^2\text{)})$
$c_T = 2.16 \times 10^{-4} \text{ 1/}^\circ\text{C}$	$(1.20 \times 10^{-4} \text{ 1/}^\circ\text{F)}$
$K_r = (k_r \rho g)/(\mu g_c) = 43.9 \text{ m/day}$	(144 ft/day)
$K_z = (k_z \rho g)/(\mu g_c) = 4.39 \text{ m/day}$	(14.4 ft/day)
$\phi = .25$	

Fluid Density Model:

<u>Temperature</u>		<u>Density</u>		<u>Actual Density</u>	
<u>°C</u>	<u>°F</u>	<u>kg/m³</u>	<u>lbm/ft³</u>	<u>kg/m³</u>	<u>lbm/ft³</u>
10.0	50.0	1000.0	62.43	999.7	62.41
12.8	55.0	999.6	62.40	--	--
15.6	60.0	998.9	62.36	999.1	62.37
18.3	65.0	998.3	62.32	--	--
20.0	68.0	998.0	62.30	998.1	62.31
21.1	70.0	997.8	62.29	998.0	62.30
23.9	75.0	997.1	62.25	--	--
26.7	80.0	996.5	62.21	996.7	62.22
29.4	85.0	995.9	62.17	--	--
32.2	90.0	995.4	62.14	995.1	62.12
35.0	95.0	994.7	62.10	--	--
37.8	100.0	994.1	62.06	994.1	62.06
40.6	105.0	993.5	62.02	--	--
43.3	110.0	993.0	61.99	991.1	61.87
46.1	115.0	992.3	61.95	--	--

48.9	120.0	991.7	61.91	988.5	61.71
51.7	125.0	991.1	61.87	--	--
54.4	130.0	990.6	61.84	985.9	61.55
57.2	135.0	989.9	61.80	--	--
60.0	140.0	989.3	61.76	983.2	61.38
62.8	145.0	988.7	61.72	--	--
65.6	150.0	988.2	61.69	980.3	61.20

Actual density is obtained from J. Hilsenrath, et al., Tables of thermal properties of gas, NBS Circular 564, 1955, International critical tables. (New York, McGraw-Hill, Inc.) reprinted in John and Haberman, 1971.

Viscosity Model (Injection and Reservoir Fluid)

<u>Temperature</u>		<u>Viscosity</u>	
<u>°C</u>	<u>°F</u>	<u>((N-day)/m²)x 10⁻⁹</u>	<u>Cp</u>
20.0	68.0	11.7	1.014
21.1	70.0	11.4	.981
26.7	80.0	9.96	.861
32.2	90.0	8.83	.763
37.8	100.0	7.88	.681
43.3	110.0	7.10	.614
48.9	120.0	6.47	.559
54.4	130.0	5.91	.511
60.0	140.0	5.43	.469
65.6	150.0	5.01	.433
71.1	160.0	4.64	.401

[TRR] = [TIR] = 68.0 °F and [VISRR] = [VISIR] = 1.014 for reference temperature, and viscosity. This table is the viscosity table used by the model to compute viscosity. Data were obtained from Streeter, 1971.

The differencing procedure is implicit in time and upwind in space on the convective term of the energy equation. Fluid allocation at the production-injection well was based on mobilities.

There are several basic differences between the CCC and INTERCOMP code parameters and domain. These are as follows:

1. One-dimensional thermal conduction transport is assumed in the overburden and underburden, while CCC uses two-dimensional aquitard properties similar to storage formation except with lower porosity and permeability. The distance from the aquifer boundary to the last boundary node in the confining layers of constant temperature is 15m for CCC and 10m for INTERCOMP.
2. Variable fluid thermal properties are allowed in the CCC code where $C_v = C_v(T)$ instead of $C_p = \text{constant}$ in the INTERCOMP code.
3. Infinite mesh extension with large node spacing is used outside the zone of thermal influence to simulate an infinite aquifer in CCC.

The formulation of the basic algorithms for the CCC code is given in papers by Sorey (1978) and Lippman, Tsang, and Witherspoon (1977).

The conceptual model will not perform well in a pressure simulation because of the axisymmetric domain assumption. The hypothetical hydraulic boundaries probably allow inflow on two sides of the aquifer if the domain is extended far enough away from the injection-production well; hence, the expected hydraulic head losses in the aquifer will be much larger than those predicted by the simulator. The relative magnitude of the pressure around the injection-production well is assumed to be the same as that found in the experiment. In addition, accurate pressure simulation requires the exact rates of injection and production rates used in the experiments which leads to using small time steps in the simulator. Therefore, no comparisons are made to pressure data obtained during the second cycle of the experiment.

Temperature results from the simulator are compared to results obtained from instrumented observation wells containing uniformly spaced ther-

mistors in the vertical direction (Figure 5-2). These wells were backfilled with sand after initial observations indicated that free convection in the wellbore caused an unnatural uniform temperature read-out with depth which was not representative of temperature in the aquifer. Figures 5-7 to 5-11 are plots of temperature vs. time in an observation well sampling of thermistor B at a depth of 4.82m (15.8 ft) beneath the top of the formation. Comparisons with (smoothed) observed, LBL simulated, and INTERCOMP simulated results are shown for well numbers 3, 2, 1, 5, 8 and 4. In Figure 5-11, asymmetric thermal response of field data is caused by a hydraulic boundary on the northwest. Well 8 is on the north side of the well field, and well 4 is on the south. In general, the INTERCOMP-derived results predict more diffusion than the LBL results, and the time of arrival of peak temperature is underpredicted by both simulations. Discrepancies between observed and simulated responses are probably due to local inhomogeneities in the storage aquifer. The effect of the hydraulic boundary in the northwest is seen by the suppressed thermal response in well 8 on the north side of the flow field when compared to well 4 on the south.

Figures 5-12 and 5-13 compare production temperatures for the first and second cycles of the experiment. In general, results from the INTERCOMP code tend to overpredict the observed temperature in both cycles.

Figures 5-14 to 5-17 show isotherms at the end of storage and after recovery for the first and second cycles. In general, as in the LBL simulation, there is a tendency to predict higher temperatures at the top and lower temperatures at the bottom when compared to field results. This suggests a higher hydraulic conductivity at the top and a lower value at the bottom.

Table 5-2 is a list of pertinent information about the energy balance. The efficiency of a recovery cycle is defined as the ratio of energy produced over the temperature of 20° C (68° F) to energy injected over the temperature of 20° C (68° F). For the first cycle, the simulated efficiency is 0.68 and the observed efficiency is 0.66. In the second cycle, the simulation predicts efficiency of 0.78 and observed efficiency was 0.76.

Differences in cumulative energy injected and produced were noted between LBL and INTERCOMP tabulations. Part of the reason for this difference appears to be caused by the variable thermal properties used by LBL and constant thermal properties by INTERCOMP. Another reason for this difference is due to the use of different base energy values used to evaluate the cumulative energy tables. For example, Tsang et al. (1980) show 0.721×10^{13} J and 0.486×10^{13} J injected and produced, respectively, during the first injection cycle. INTERCOMP results show 0.809×10^{13} J and 0.547×10^{13} J for the same respective parameters. The efficiency ratios predicted by Tsang et al. (1981) are 0.67 and 0.77 for the first and second cycles, respectively. Other possible causes of this discrepancy are discussed in the discussion section.

Table 5-2. Energy Budget

Initial total water in place = 2.071×10^8 kg (4.5648 $\times 10^8$ lbm)
 (G) Initial total energy in place = 1.754×10^{13} J (1.6625 $\times 10^{10}$ Btu)

First Cycle:

End of first cycle - Cumulative time = 170.83 days

Cumulative water injected = 5.425×10^7 kg (1.196 $\times 10^8$ lbm)
 Cumulative energy injected = 1.262×10^{13} J (1.196 $\times 10^{10}$ Btu)

Cumulative water produced = 5.498×10^7 kg (1.212 $\times 10^8$ lbm)
 Cumulative energy produced = 1.007×10^{13} J (9.543 $\times 10^9$ Btu)

Base temperature $T_o = 20.0^\circ$ C (68° F)
 Base pressure $p_o = 3.751 \times 10^5$ N/m² (54.4 psi)

Enthalpy of fluid at $(T_o, p_o) = 8.509 \times 10^4$ J/kg (36.58 Btu/lbm)

Cumulative energy injected at base enthalpy = 4.616×10^{12} J
 (4.375 $\times 10^9$ Btu)

Cumulative energy produced at base enthalpy = 4.677×10^{12} J
 (4.433 $\times 10^9$ Btu)

(A) Cumulative energy injected above base enthalpy = 8.003×10^{12} J
 (7.585 $\times 10^9$ Btu)

(B) Cumulative energy produced above base enthalpy = 5.391×10^{12} J
 (5.110 $\times 10^9$ Btu)

Efficiency = $5.110 \times 10^9 / 7.585 \times 10^9 = .67$
 Efficiency observed = .66

(D) Cumulative energy loss to confining layers =
 1.019×10^{12} J (9.655 $\times 10^8$ Btu)

(F) Total energy in place = 1.912×10^{13} J (1.812 $\times 10^{10}$ Btu)
 Total water in place = 2.070×10^8 kg (4.564 $\times 10^8$ lbm)

Total energy in place at base enthalpy = 1.762×10^{13} J (1.670 $\times 10^{10}$ Btu)
 Total energy in place above base enthalpy = 1.503×10^{12} (1.425 $\times 10^9$ Btu)

(A) - (B) = (C) =

Unrecovered energy at end of 1st cycle = 2.611×10^{12} J (2.475 $\times 10^9$ Btu)

(C) - (D) = (E) =

Unrecovered energy in reservoir at end of 1st cycle =
 1.593×10^{12} J

(1.510 $\times 10^9$ Btu)

(F) - (G) = (H)

Energy in place (above base enthalpy) at end of 1st cycle =
 $1.577 \times 10^{12} \text{ J}$ $(1.495 \times 10^9 \text{ Btu})$
 Energy Balance = $(H)/(E) = .99$ (Energy is balanced)

Second Cycle:

Second Cycle begins at cumulative time = 191.0 days
 Energy balance evaluated at cumulative time = 372.3 days
 Time since beginning of second cycle = 181.3 days

Cumulative water injected = $1.117 \times 10^9 \text{ kg}$ $(2.463 \times 10^8 \text{ lbm})$
 Cumulative energy injected = $2.603 \times 10^{13} \text{ J}$ $(2.467 \times 10^{10} \text{ Btu})$

Cumulative water produced = $1.214 \times 10^8 \text{ kg}$ $(2.676 \times 10^8 \text{ lbm})$
 Cumulative heat produced = $2.240 \times 10^{13} \text{ J}$ $(2.123 \times 10^{10} \text{ Btu})$

Total water injected - second cycle = $5.747 \times 10^7 \text{ kg}$ $(1.267 \times 10^8 \text{ lbm})$
 Total energy injected - second cycle = $1.341 \times 10^{13} \text{ J}$ $(1.271 \times 10^{10} \text{ Btu})$

Total energy injected at base enthalpy - second cycle =
 $4.890 \times 10^{12} \text{ J}$ $(4.635 \times 10^9 \text{ Btu})$
 Total energy produced at base enthalpy - second cycle =
 $5.650 \times 10^{12} \text{ J}$ $(5.335 \times 10^9 \text{ Btu})$

- (I) Total energy injected above base enthalpy - second cycle =
 $8.520 \times 10^{12} \text{ J}$ $(8.075 \times 10^9 \text{ Btu})$
 (J) Total energy produced above base enthalpy - second cycle =
 $6.684 \times 10^{12} \text{ J}$ $(6.335 \times 10^9 \text{ Btu})$

Efficiency = $6.335 \times 10^9 / 8.075 \times 10^9 = .78$
 Efficiency observed = .76

- Cumulative heat loss by conduction at 191 days =
 $1.008 \times 10^{12} \text{ J}$ $(9.558 \times 10^8 \text{ Btu})$
 (L) Cumulative heat loss by conduction at 372.3 days =
 $2.192 \times 10^{12} \text{ J}$ $(2.078 \times 10^9 \text{ Btu})$

Cumulative heat injected above base enthalpy =
 $1.652 \times 10^{13} \text{ J}$ $(1.566 \times 10^{10} \text{ Btu})$
 Cumulative heat produced above base enthalpy =
 $1.207 \times 10^{13} \text{ J}$ $(1.144 \times 10^{10} \text{ Btu})$

Average efficiency = $1.144 \times 10^{10} / 1.566 \times 10^{10} = .73$

- (N) Total energy in place = $1.979 \times 10^{13} \text{ J}$ $(1.876 \times 10^{10} \text{ Btu})$
 Total water in place = $2.070 \times 10^8 \text{ kg}$ $(4.564 \times 10^8 \text{ lbm})$

Total energy in place at base enthalpy = $1.761 \times 10^{13} \text{ J}$ $(1.670 \times 10^{10} \text{ Btu})$
 Total energy in place above base enthalpy = $2.179 \times 10^{12} \text{ J}$ $(2.065 \times 10^9 \text{ Btu})$

(I) - (J) + (E) = K =
 Unrecovered energy at end of 2nd cycle = $3.429 \times 10^{12} \text{ J}$ $(3.250 \times 10^9 \text{ Btu})$

(K) - (L) + (D) = M =
Unrecovered energy in reservoir at end of 2nd cycle =
2.256 x 10¹² J (2.138 x 10⁹ Btu)
(N) - (G) = (O) =
Energy in place (above base enthalpy) at end of 2nd cycle =
2.258 x 10¹² J (2.140 x 10⁹ Btu)

Energy balance = (O)/(M) = 1.001 (Energy is balanced)

Figure 5-7. Simulation comparisons for 9 meters (29 ft) radial distance at thermistor B.

Figure 5-8. Simulation comparisons for 18 meters (59 ft) radial distance at thermistor B.

Figure 5-9. Simulation comparisons for 21 meters (69 ft) radial distance at thermistor B.

Figure 5-10. Simulation comparisons for 37 meters (121 ft) radial distance at thermistor B.

Figure 5-11. Comparisons for simulation at 45 meters (148 ft).

Figure 5-12. Production temperature comparisons during the first cycle.

Figure 5-13. Production temperature comparisons during the second cycle. The arrow signifies time at which the second cycle efficiency is computed.

TEMPERATURE CONTOURS

Figure 5-14. Temperature contour comparisons between LBL, INTERCOMP, and observed results. The time is 129.73 days, at the end of storage in the first cycle.

TEMPERATURE CONTOURS

Figure 5-15. Temperature contour comparisons at the end of simulation of first cycle. Time is 170.83 days.

TEMPERATURE CONTOURS

LMOB After second cycle injection, time-63.38 days, Cum. time=254.38 days.

Figure 5-16. Temperature contour comparisons at the end of injection for the second cycle. Time is 63.38 days after the start of second cycle.

TEMPERATURE CONTOURS

LMOB after second cycle recovery, time=181.3 days, Cum. time=372.3 days

Figure 5-17. Temperature contour comparisons after production in the second cycle. Time is 181.30 days since the beginning of second cycle of simulation.

PART 6

DISCUSSION AND CONCLUSIONS

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CODE CHANGES

Results of code response to the analytical solution appear to prove the accuracy of the code. Some of the comparisons between CDC and IBM results seem to prove otherwise when looking at a single parameter like heat loss. However one should remember that the CDC simulation was conducted using another almost identical code and that the simulation comparisons took place over a very small time span involving very small quantities of energy loss compared to total energy in the reservoir. Comparisons with independent analytical and numerical solutions over longer time periods with larger relative mass and energy interchange appear to verify code accuracy. The major cause of output differences were machine dependent errors in the balance algorithms.

A number of minor errors were found in the code that have negligible effects on to the test problems and were never detected in earlier code verification studies. A number of changes were made to make parameter computations consistent with others found in the code. New convenience options were adapted to the code from the INTERA (1979) version. One such option is the manual radial grid generator which allows the user to insert nodes at exact locations of field observation wells. This is a difficult task in the unmodified code because a radial mesh configuration assumed mesh boundary values (rb) that are allocated by

$$rb_{i+1}/rb_i = C$$

where C is a constant.

The version of the code released by INTERCOMP through the National Technical Information Service (NTIS) does not appear to be identical to the code used to demonstrate code capability in the original document released in 1976, because the example printout is not possible with the version received from NTIS. Corrections to the output have been implemented on the updated version of the code.

CODE PHYSICAL INPUT PARAMETERS

Overall, the INTERCOMP DWDM is written very well with much computer and numerical insight for solving solute waste disposal in deeply buried formations. Hydraulic porous media parameters have the most input flexibility. For example, porosity (ϕ) and hydraulic conductivity (K) can be entered on a regional basis. In contrast, thermal properties are less flexible. For an illustration, the present code allows treatment of thermal conductivity of the medium as a constant, with only directional variation, and makes no input provisions for thermal conductivity changes due to changes in rock type or porosity; however, the code stores individual thermal conductivity data for each block for the x-, y-, and z-directions. With very minor input modifications, the thermal conductivity of the rocks can be entered like hydraulic conductivity and can be computed by one of three models listed below:

1. arithmetic mean model (parallel conduction);

$$K_m = \phi K_w + (1 - \phi) K_R \quad (6-1)$$

2. geometric mean model:

$$K_m = K_w^\phi \cdot K_R^{(1-\phi)} \quad (6-2)$$

3. harmonic mean model (series conduction):

$$\frac{1}{K_m} = \frac{(1-\phi)}{K_R} + \frac{\phi}{K_w} \quad (6-3)$$

where K_m is the effective thermal conductivity of the porous medium and K_R and K_w are thermal conductivities of the rock and water (Bear, 1972; Reffstrup, 1979). Reffstrup shows that the best representative thermal conductivity is the geometric mean model for porous media.

Like the thermal conductivity, the heat capacity of water at constant pressure (C_p) is entered as a constant. Rock heat capacity per unit volume (ρC_p)_R is entered as a constant, implying incompressible rock. The constant heat capacity of water is a good assumption provided that the temperature of the fluid remains less than 99° C at 1 atmosphere or greater pressure (Dorsey, 1940, p. 259). Density of the rock is not always treated as a constant. This discrepancy is shown in equation (2-29) where $\phi_o c_R \delta p$ represents the change in rock fraction of porosity caused by a change in pressure. Slightly compressible rock is also assumed in calculating the pore volume in equation (3-7) for computing fluid mass in place. The assumption of constant (ρC_p)_R is ideal, because, like thermal conductivity, heat capacity per unit volume of rock for a fluid reservoir is generally unknown. The above assumption is expected to be valid because the compressibility of rock is small, usually ranging from 10^{-6} to 10^{-11} m²/N (Freeze and Cherry, 1979, p. 55).

If the wellbore model is being used and the energy equation is being solved, horizontal aquifer thermal conductivity is used in the line source heat loss calculation in the wellbore. Wellbore thermal conductivity is related to aquifer thermal conductivity by

$$K_{wb} = \sqrt{2} \sqrt{(K_x)^2 + (K_y)^2} \quad (6-4)$$

where K_x and K_y are reservoir thermal conductivity in the x and y directions, respectively. The heat capacity of the matrix that surrounds the wellbore is set independent of previous input by a separate entry for thermal diffusivity, $(K_{wb}/(\rho C_p)_{wb})$.

The operations of the wellbore heat loss model use an approximate solution of the thermal diffusivity equation. The model does not keep track of temperature influences from aquifer and overburden layers. It assumes a constant heat flux in or out of the wellbore and bases its solution on a time function which begins at the start of simulation with an initial temperature profile assigned by the vertical temperature table. Therefore, the model is most accurate when a fluid of constant temperature is injected or produced for long periods of time in a long wellbore.

The INTERCOMP simulator is designed to handle fully saturated aquifers. The output pressure tables are given in absolute values. For simulations without the use of the wellbore model, the aquifer pressure may be at gage pressure by establishing a zero pressure at the surface and measuring the initial pressure [PINIT] with respect to the zero surface pressure. However, when the wellbore model is in effect, the atmospheric pressure entry into the wellbore model is in effect. The atmospheric pressure entry into the wellbore model is [PBASE], which is used to establish a base pressure for the wellbore.

model. Therefore, the value of [PINIT] should be based on one atmospheric pressure or dependent upon what is used in [PBASE].

In general, the user should base [PINIT] and [PBASE] on absolute pressure at the surface especially when solving the energy equation because the base internal energy and enthalpy calculations use Tables 2-1 and 2-2 which are dependent upon absolute pressure input. For the purpose of simulations attempted in this study where pressures were gage pressure for all problems except the radial test problem in Part 3, the expected errors are in the order of a few tenths of a percent because enthalpy is a weak function of pressure in a low pressure liquid dominated problem.

The newer version of the INTERCOMP code released in 1979 has options for free water surface (restricted to uppermost finite difference block layer) in the aquifer, with vertical recharge, solute adsorption, and single component radioactive decay. When a free surface option is chosen, the model will not solve the energy equation. As a result, this newer version adds very little additional user flexibility for ATEs simulations. The energy equation is not solved because the heat storage and transport in partially saturated blocks must be separated into dry and wet parts.

MODEL CONSTRUCTION AND OPTION DATA

Parts of the code were constructed from existing software; hence, the code contains a number of independent steps and internal labels which have no meaning. A few of these redundant steps and labels were removed when updating the code.

An option which appears to set the bottom-hole pressure constant is found in the wellbore source allocation option. This option can be accessed

by setting [IINDW1] = -4 and specifying bottom-hole pressure through [BHP]. No instructions for its use were found in the original document, and initial tests of this option proved it to be unreliable. Therefore, its use requires some caution. This option was left in the code and is still accessible by specifying [IINDW1] = -4. The accompanying error message for [IINDW1] is extended to ± 4 instead of ± 3 as specified in error #30 ([IINDW1] is out of range) so the above option is functional in the modified version. Since the use of this option was unreliable, no notation of its existence is given in the user input and error messages in Appendix D. This option sets the bottom-hole pressure as [BHP] and computes a flow rate to achieve [BHP]; hence, the value of the volumetric source rate has no meaning.

The use of the various well specification options [IINDW1] require some explanation. The INTERCOMP code tends to allocate flow rates that are not the same flow rates the user has specified. The magnitude of the discrepancy depends upon which [IINDW1] option is specified. These errors occur partially because of iteration errors that occur during the flow allocation calculations used to preserve solution stability around the source.

The following is an example based on the solution of the one-dimensional flow problem by Brenner (1962) and Coats and Smith (1964). Injection fluid density is 62.3 lbm/ft³ and injection rate is 0.1 ft³/day, or 6.23 lbm/day through a .305 x .305 m cross-section "tube." The allocated flow rates by the model are given as a function of time in Table 6-1 when the simulator is assigned a constant injection rate specified by the user before the first time step. Table 6-1 was the result of using high hydraulic conductivities (2000 ft/day) and low flow rates to force the bottom-hole (p_{bh}) and grid block pressure (p_g) difference to be a small and inaccurate difference between two

large numbers; hence, flow allocation by pressure drop ($p_{bh} - p_g$) between the wellbore and the grid blocks is inaccurate. When the well index and hydraulic conductivities are decreased, the allocation calculations become more precise because $p_{bh} - p_g$ increases in magnitude.

Another cause of allocation error comes from the "drifting" of the flow allocation rate in the explicit term of the semi-implicit source allocation. This is caused by tolerance errors in the flow rate adjustment for the explicit flow rate to achieve desired rates in [ITER].

In general, the INTERCOMP flow rates tends to be slightly less than user specified flow rates when using [IINDW1]=1 for flow allocation by mobilities by 1 to 2% for both production and injection wells. Allocation by pressure drop and mobilities, and semi-implicit allocation tend to follow similar but less rigorous rules with larger differences between the allocated and user specified flow rates. Therefore the user should check the allocation rates in the output table, especially when using the allocation by pressure drop and mobilities option, and moreso when using the semi-implicit option.

In a number of test problems, the few percentage errors in the allocation show up as small and minor contributions to actual node pressure, temperature, and concentration output. For the example problem (see Table 6-1) addressed earlier, where the temperature of the injection fluid was at 100° F and initial reservoir temperature was 70° F, with $K=2000$ ft/day, the maximum node temperature difference between allocation option of [IINDW1]=1 (allocation by mobilities) and -2 (allocation by pressure drop and mobilities and semi-implicit source option), problems at time=700 days was .3° F. A discussion on the source allocation technique is given in Appendix C.

The [EPS] option for tolerance on calculating temperature from given values of enthalpy and pressure does not work. The value of [EPS] is set at 0.001 in the code and has been adequate. If the user desires the above option, the read statement still contains a position to read [EPS]; however, the user would have to modify the fix common block to transfer [EPS] to where it is needed.

The present version of the code contains both double precision variables (REAL*8) and single precision variables (REAL*4). The means of data storage is not as efficient as the original code because of the existence of a REAL*8 or double precision array, followed by REAL*4 arrays in the variable common blocks. Optimal storage efficiency can be obtained by knowing the length of the REAL*8 array before compiling the main program, as follows:

$$[IDLAST] = 3*[NB] + 2*[NABLMX] + 1$$

where [IDLAST] is the size of the REAL*8 arrays required, NB = number of x-blocks times number of y-blocks times number of z-blocks, and [NABLMX] is the maximum number of aquifer influence blocks. Additional information about redimensioning of the code is given in appendix D.

Table 6-1. Flow Allocation Comparisons

<u>Time (Days) Well Specification [IINDW1]</u>			
<u>K=2000. ft/day</u>	<u>1</u>	<u>2</u>	<u>-2</u>
.10 days	6.053 lbm/day	6.053 lbm/day	6.053 lbm/day
.20	6.053	5.039	6.023
10.0	6.053	5.058	5.858
50.0	6.053	5.282	5.575
100.0	6.053	5.321	5.477
<u>K=500. ft/day</u>			
.10	6.053	6.053	6.053
.20	6.053	5.908	6.060
10.0	6.053	5.879	6.052
50.0	6.053	5.903	6.038
100.0	6.053	5.911	6.022
[IINDW1] = 1 Flow allocation by mobilities only and explicit source.			
[IINDW1] = 2 Flow allocation by mobilities and pressure drop and explicit source.			
[IINDW1] = -2 Flow allocation by mobilities and pressure drop and semi-implicit source.			

Parts of the model were not studied in detail. The least amount of time was spent in learning the details of the solvers [GAUS3D] and [L2SOR] and the associated subprograms [ORDER], [LSORX], [LSORY], and [LSORZ]. These subprograms are also used in a number of related petroleum reservoir and environmental simulators produced by INTERCOMP and INTERA.

The wellbore heat loss model was not tested except for running a test problem documented by INTERCOMP. Options such as specified surface pressure and specified rate ([IINDW1 = ± 3]) were not tested and are assumed to be correct. A summary about the operations of the wellbore model and its related input are given in Appendix C.

The DWDM is not well suited for computing only the pressure equation. There are other more efficient and more manageable codes to do just that, because the INTERCOMP code prepares arrays and makes decisions for energy and solute equations regardless of the code use.

CONCLUSION

Code comparisons with simplified numerical and analytical solutions appear to confirm the authenticity of code results. Discrepancies noted in fluid mass and energy balance were primarily caused by machine limitations. A number of minor errors were found in the code. These probably were not detected earlier because these errors are either small or are parts of options not used in earlier test problems.

Simulated results from INTERCOMP were compared with the Lawrence Berkeley Laboratory CCC code. Node temperature results compare fairly well with CCC results; however, computations of cumulative energy in and energy out are different. These differences were partially attributed to the use of a

less accurate means of computing energy by the INTERCOMP code. The aquifer influence function infinite aquifer option has proven to be a very useful tool to save on storage and machine time. Results from the use of one-dimensional heat conduction heat loss computation to two-dimensional heat conduction in CCC is inconclusive because the length of the last block where temperature is held constant is 10m for the INTERCOMP simulator and 15m for the LBL.

Energy recovery ratios and prediction of recovery temperatures compared well with CCC and observed results. In general, both recovery ratios for first and second cycles and recovery temperature were slightly overpredicted.

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APPENDIX A
TAPE DOCUMENTATION

The magnetic tape library consists of three sets of data. The first data set is INTER. This contains the source listing of the modified version of the INTERCOMP code enclosed in card format of 80 characters in length. This data set can be read by using the enclosed read-write FORTRAN program. The second set of data are input card decks of 80 characters in length (LRECL = 80) for the various test problems. This data set consists of copies of input to simulations of Parts 3, 4 and 5. A number of input files may contain slightly different data than those used in Part 4; hence output obtained may not duplicate output given in Part 4. In general nodal results obtained are very close to responses observed in Part 4. A number of the test problems involved several simulations. Only one of each test is enclosed in the tape library. The third set of data are the output obtained using the above mentioned input cards having 132 characters per printed line. The tape library is given in Table A-1.

Table A-1--TAPE LIBRARY

<u>File Number</u>	<u>Data Set Name</u>	<u>Description</u>
1	INTER	Modified program
2	ZTEST	INTERCOMP test problem input
3	ZTHEIS	Theis test problem input
4	ZSEST	Shape test problem input
5	ZHOPS	Hoopes and Harleman input
6	ZONED	Coats and Smith input
7	ZAVDR	Avdonin radial input
8	ZAVDRL	Avdonin radial-linear input
9	ZAVDL	Avdonin linear 1-D input

10	GRING1	Gringarten and Sauty input (0-.2d)
11	GRING2	Gringarten and Sauty input (.2-30d)
12	GRING3	Gringarten and Sauty input (30-500d)
13	LMOB1	Mobile experiment (0-13.79d)
14	LMOB2	Mobile experiment (13.79-129.73d)
15	LMOB3	Mobile experiment (129.73-170.83d)
16	LMOB4	Mobile experiment (170.83-254.38d)
17	LMOB5	Mobile experiment (254.38-400d)
18	ZTES0	INTERCOMP test problem output
19	ZTHEI0	Theis test problem output
20	ZSES0	Shape test problem output
21	ZHOPO	Hoopes and Harleman output
22	ZONEO	Coats and Smith output
23	ZAVDRO	Avdonin radial output
24	ZAVDRLO	Avdonin radial-linear grid output
25	ZAVDL10	Avdonin linear 1-D output
26	GRING1	Gringarten and Sauty output (0-2d)
27	GRING2	Gringarten and Sauty output (.2-30d)
28	GRING3	Gringarten and Sauty output (30-500d)
29	LMOB10	Mobile experiment (0-13.79d)
30	LMOB20	Mobile experiment (13.79-129.73d)
31	LMOB30	Mobile experiment (129.73-170.83d)
32	LMOB40	Mobile experiment (170.83-254.38d)
33	LMOB50	Mobile experiment (254.38-400.d)

File numbers 2 to 17 are input files, and files 18 to 33 are output files.

The above list of the modified version of the INTERCOMP program, input data cards, and output files was written to tape by PROGRAM 1 and can be recovered from tape by PROGRAM 2. The listing of these programs is given below.

Most of the items in the code output are self-explanatory. A large part of the initial code output is a confirmation of input data. A number of the output summary data are abbreviated and require clarification. These are listed below.

[ITIME] =	Number of time steps
[ITNS] =	Number of outer iterations in [ITER] at [ITIME]
[MBW] =	Mass balance on aquifer fluid evaluated like equations (3-1) and (3-2) or fluid mass in aquifer at current time + Fluid produced + Initial fluid in aquifer (divided by) Fluid injected + Fluid influx the across aquifer boundaries
[MBCOMP] =	Mass balance on solute, like equations (3-1) and (3-2)

[HEATBL] =	Energy balance, like equations (3-1) and (3-2)
[TOTWP] =	Total water produced up to current time [TIME]
[TOTCP] =	Total component produced up to current time [TIME]
[TOTHP] =	Total heat produced up to current time [TIME]
[MM] =	Million, or [MMBTU] = million BTU
[TOTWI] =	Total water injected up to current time
[TOTCI] =	Total component injected up to current time
[TOTHI] =	Total heat injected up to current time
[TWIP] =	Current total water in place
[TCIP] =	Current total component in place
[THIP] =	Current total heat in place
[PAVG] =	Pore volume weighted average pressure calculated at datum by correcting with $-\rho_o gh/g_c$, where ρ_o is resident fluid density at [PINIT] and T_O , and h is positive downward, measured from datum to top grid blocks.
[HEAT LOSS] =	Cumulative heat loss to overburden and underburden.
[DPMAX] =	Maximum grid block pressure change over a time step, δp Locations are given in parenthesis as positions I, J, K block location
[DCMAX] =	Maximum concentration change, δC
[DTEMPMAX] =	Maximum temperature change, δT
[CUM WATER INFLUX] =	Cumulative component influx through the external boundaries govern by aquifer influence functions. Negative influx indicate water efflux.
[CUM COMP. INFLUX] =	Cumulative component influx
[CUM HEAT INFLUX] =	Cumulative heat influx
[GRID BLOCK PRESS] =	Grid block pressure, psi. The pressure in the grid block in the uppermost layer open to well, p_g .
[FLWG BHP] =	Flowing well bottom-hole pressure, [FWP], psi
[FLWG WHDP] =	Flowing well head pressure, [WHP], psi

[BH TEMP] = Bottom-hole temperature, °F

[WH TEMP] = Wellhead temperature, °F

Pressure output are given in psia in the listing; however, the values printed in all cases with the exception of the listing in ZTESO are actually in psi. The datum pressure was adjusted so that zero gauge pressure existed at the surface.

All input data decks for the test problems assume the existence of an output file on unit 12, and all problems were executed from an existing load module. Both the Gringarten and Sauty and Mobile experiment test problems were run using a series of restarts, and therefore require the existence of restart tapes on unit 8 for output and unit 4 for input.

The technology transfer tape is written in EBCDIC, with a logical record of 80, a block size 1600 for source, and input data decks (files 1 to 17). Output files have logical record length of 132 and block size of 2640. The tape density is 1600 bytes per inch.

```

1.      //      JOB(.,18),'NAME',MSGLEVEL=(1,1),MSGCLASS=A,
2.      // NOTIFY=VTIGO,TIME=(,9),CLASS=S
3.      // EXEC FORGICLG,REGION=220K
4.      //FORT.SYSIN DD *
5.      C
6.      C
7.      C   THIS PROGRAM COPIES FROM DISK TO TAPE.
8.      C
9.      C
10.     DIMENSION A(33)
11.     DATA DLIMIT/'$$$$'/
12.     C
13.     C   FOR PRINTED OUTPUT, SET IOUT=1, OTHERWISE SET IOUT=0.
14.     C   FOR OUTPUT LISTING TRANSFER, SET ITYPE=1, OTHERWISE ITYPE=0.
15.     C   INPUT UNIT=12.
16.     C   OUTPUT UNIT=13.
17.     C   THE LAST CARD CONTAINS DELIMITER OF '$$$$'.
18.     C   THIS CARD INDICATES END OF DATA SET.
19.     C   NOTE THIS PROGRAM ASSUMES FOUR CHARACTERS PER WORD DATA STRUCTURE.
20.     C
21.     REWIND 12
22.     IOUT=0
23.     ITYPE=0
24.     IL=20
25.     IF(ITYPE.EQ.1)IL=33
26.     ILINE=0
27.     DO 10 I=1,42000
28.     READ(12,8) (A(J),J=1,IL)
29.     8   FORMAT(33A4)
30.     IF(A(1).EQ.DLIMIT)GO TO 11
31.     WRITE(13,9)(A(J),J=1,IL)
32.     IF(IOUT.EQ.1)WRITE(6,7) (A(J),J=1,IL)
33.     7   FORMAT(1H ,33A4)
34.     9   FORMAT(33A4)
35.     ILINE=ILINE+1
36.     10  CONTINUE
37.     11  WRITE(13,9)(A(J),J=1,IL)
38.     WRITE(6,12) ILINE
39.     12  FORMAT(1H0,'NUMBER OF LINES COPIED = ',15)
40.     C
41.     C   FOR SOURCE LISTING AND CARD INPUT LET LRECL=80.
42.     C   FOR OUTPUT LISTING LET LRECL=132.
43.     C   SET BLKSIZE AS SOME MULTIPLE OF LRECL.
44.     C
45.     STOP
46.     END
47.     //GD.FT12F001 DD DSN=USER.Y7R51.RUN2,UNIT=CDISK,DISP=OLD
48.     //FT13F001 DD DSN=LMQ84,UNIT=TAPE,VOL=SER=C13259,
49.     // LABEL=(17,EXPDT=99365),
50.     // DISP=(NEW,CATLG),DCB=(RECFM=FB,LRECL=80,BLKSIZE=1600)
51.     /*

```

```

1.      //      JOB(,,9), 'NAME', MSGLEVEL=(1,1), MSGCLASS=A,
2.      // NOTIFY=VTIG0, TIME=(,8), CLASS=S
3.      //CREATE EXEC PGM=IEFBR14
4.      //DD1 DD DSN=USER.Y7851.PROG, UNIT=CDISK,
5.      // DISP=(NEW,CATLG), DCB=(RECFM=FB, LRECL=80, BLKSIZE=1600),
6.      // SPACE=(TRK,(5,1))
7.      // EXEC FORGICLG, REGION=220K
8.      //FORT.SYSIN DD *
9.      C
10.     C
11.     C THIS PROGRAM COPIES FROM TAPE TO DISK.
12.     C
13.     C
14.     C      DIMENSION A(33)
15.     C      DATA DLIMIT/'$$$$'/
16.     C
17.     C      FOR PRINTED OUTPUT, SET IOUT=1, OTHERWISE SET IOUT=0.
18.     C      FOR OUTPUT LISTING TRANSFER, SET ITYPE=1, OTHERWISE ITYPE=0.
19.     C      INPUT UNIT=12.
20.     C      OUTPUT UNIT=13.
21.     C THE LAST CARD CONTAINS DELIMITER OF '$$$$'.
22.     C THIS CARD INDICATES END OF DATA SET.
23.     C THIS PROGRAM ASSUMES FOUR CHARACTERS PER WORD DATA STRUCTURE.
24.     C
25.     C      IOUT=0
26.     C      ITYPE=0
27.     C      REWIND 12
28.     C      IL=20
29.     C      IF (ITYPE.EQ.1) IL=33
30.     C      ILINE=0
31.     C      DO 10 I=1, 20000
32.     C      READ(12,8) (A(J), J=1, IL)
33.     C      8      FORMAT(33A4)
34.     C      IF (A(1).EQ.DLIMIT) GO TO 11
35.     C      WRITE(13,9) (A(J), J=1, IL)
36.     C      IF (IOUT.EQ.1) WRITE(6,7) (A(J), J=1, IL)
37.     C      7      FORMAT(1H ,33A4)
38.     C      9      FORMAT(33A4)
39.     C      ILINE=ILINE+1
40.     C      10     CONTINUE
41.     C      11     WRITE(13,9) (A(J), J=1, IL)
42.     C      WRITE(6,12) ILINE
43.     C      12     FORMAT(1H0, 'NUMBER OF LINES COPIED = ', I5)
44.     C
45.     C FOR SOURCE LISTING AND CARD INPUT LET LRECL=80.
46.     C FOR OUTPUT LISTING LET LRECL=132.
47.     C SET BLKSIZE AS SOME MULTIPLE OF LRECL.
48.     C
49.     C      STOP
50.     C      END
51.     //GO.FT13F001 DD DSN=USER.Y7851.PROG, UNIT=CDISK, DISP=OLD,
52.     // DCB=(RECFM=FB, LRECL=80, BLKSIZE=1600)
53.     //FT12F001 DD DSN=INTER, UNIT=TAPE, VOL=SER=C12171, LABEL=5,
54.     // DISP=OLD, DCB=(RECFM=FB, LRECL=80, BLKSIZE=1600)
55.     /*

```

APPENDIX B

APPENDIX B
EQUATION DERIVATION DETAILS

This section provides details to support some of the relationships used in the code. Items provided here are unimportant to a casual user of the code. Details about overburden and underburden conduction and the wellbore heat loss model are provided in this section. Insufficient details in the original document warrant further explanation about these areas of the code, especially for a user who is interested in a heat transfer problem.

HEAT LOSS TO OVERBURDEN AND UNDERBURDEN

The basic discussion here is restricted to the overburden problem because both the underburden and overburden are treated identically. The generalized problem is best described by:

$$\nabla \cdot (K_{ob} \nabla T) = \frac{\partial (\rho C_p T)}{\partial t} \quad (B-1)$$

For 1-dimension homogeneous space, the problem simplifies to

$$K_{ob} \frac{\partial^2 T}{\partial z^2} = (\rho C_p)_{ob} \frac{\partial T}{\partial t} \quad (B-2)$$

with initial and boundary conditions of

$$\begin{aligned} t = 0 & \quad T(z, 0) = T_0(z) \\ z = 0 & \quad T(0, t) = T_a(t) \\ z = \infty & \quad T(\infty, t) = T_0(z) \end{aligned} \quad (B-3)$$

where $z = 0$ is the top of the aquifer surface and T_a refers to the temperature of the aquifer contact surface. The overburden is treated like a semi-infinite medium, which is closed to heat flow in the lateral direction.

This problem is solved using a central difference in space and implicit (in time) finite difference approximation in a finite thickness overburden, so equation (B-2) is written as

$$K_k^* T_{k-1}^{n+1} - [K_k^* + K_{k-1}^*] T_{k-2}^{n+1} + K_{k-1}^* T_{k-3}^{n+1} = \frac{(\rho C_p)_{ob}}{\Delta z_{k-1} \Delta t} [T_{k-2}^{n+1} - T_{k-2}^n] \quad (B-4)$$

where

$$K_k^* = \frac{K_{ob}}{\Delta z_k^*}.$$

The definition of the discrete variables are given in Figure B-1. The numbering scheme used is identical to the program, so the variable array coefficients are identical to those in the code. In Figure B-1 the user specified block size, defined as $[DZOB(K)]$ is represented by ΔZ_k . The code node spacing is ΔZ_k^* . Variable K_k^* is equivalent to $[TZOB(K)]$, and T_k is $[TOB(M,K)]$. The value for the K_5^* dummy term is equated to K_4^* . The value $[TOBI]$ is the constant temperature value at the boundary.

Equation (B-4) can be rewritten as

$$-K_k^* T_{k-1}^{n+1} + [K_k^* + K_{k-1}^* + \frac{(\rho C_p)_{ob}}{\Delta z_{k-1} \Delta t}] T_{k-2}^{n+1} - K_{k-1}^* T_{k-3}^{n+1} = \frac{(\rho C_p)_{ob}}{\Delta z_{k-1} \Delta t} T_{k-2}^n \quad (B-5)$$

Figure B-1. Finite difference block schematic for overburden layers.

so that all the unknown T_k^{n+1} terms are on the left-hand side. This equation can be solved using the Thomas Algorithm. The basic form after dropping the (n+1) superscript for unknowns is

$$A_{k-2} T_{k-1} + B_{k-2} T_{k-2} + C_{k-2} T_{k-3} = D_{k-2} \quad (B-6)$$

The problem is solved by assuming the following relationships

$$T_{k-3} = E_{k-1} T_{k-2} + F_{k-1} \quad (B-7)$$

and

$$T_{k-2} = E_k T_{k-1} + F_k \quad (B-7-a)$$

After substitution of equation (B-7) in equation (B-6) and simplifying and writing the result in the form of equation (B-7-a), the resultant recursion formulas are obtained

$$E_k = \frac{K_k^*}{K_k^* + K_{k-1}^* + \frac{(\rho C_p)_{ob}}{\Delta z_{k-1} \Delta t} - E_{k-1} K_{k-1}^*} \quad (B-8)$$

$$F_k = \frac{\frac{(\rho C_p)_{ob}}{\Delta z_{k-1} \Delta t} T_{k-2}^n + K_{k-1}^* F_{k-1}}{K_k^* + K_{k-1}^* + \frac{(\rho C_p)_{ob}}{\Delta z_{k-1} \Delta t} - E_{k-1} K_{k-1}^*} \quad (B-8-a)$$

which are equivalent to the $[F(K)]$ and $[E(K)]$ variables found in heat loss calculations. The $[UOB(K)]$ variable is equivalent to the denominator of equations (B-8) and (B-8-a) in the heat loss calculations in the $[PRINT2]$ and $[COEFF]$ subroutines. The thermal transmissibility K_k^* and storage term

$\rho C_p / \Delta z_k \Delta t$ are equivalent to [TZOB(K)] and [CPOB(K)], respectively.

Equations (B-8) and (B-8-a) relate knowns E_{k-1} and F_{k-1} to the unknowns E_k and F_k .

The overburden temperature is obtained by solving for F_k and E_k from $k = 3$ to the number of overburden blocks, and T_k is obtained from equation (B-7-a) with $k = \text{number of overburden blocks minus one to } k \text{ equals one}$.

Heat loss is calculated in two phases in subroutine [COEFF]. The first component of the heat loss calculation assumes no change in the boundary temperature at $z = 0$ over the period between the time steps (t^n to t^{n+1}) so the boundary conditions are

$$\begin{aligned} T_1(z, t) &= T_1(0, t) = \text{constant} & t^n \leq t \leq t^{n+1} \\ T_1(h, t) &= T_0 \end{aligned} \quad (B-9)$$

with the initial condition as the previous temperature profile from the t^n time and h is a finite length value corresponding to the position of the last temperature node where the temperature is held constant at [TOBI]. The second component is determined using the following boundary conditions

$$\begin{aligned} T_2(0, t) &= 1.0^\circ\text{F} & t^n \leq t \leq t^{n+1} \\ T_2(h, t) &= 0.0^\circ\text{F} \end{aligned} \quad (B-10)$$

The initial condition for this case assumes a zero degree temperature profile because $\delta T = 0$ initially. Boundary conditions equation (B-10) is applied to equation (B-2) to calculate the additional heat loss per degree change in temperature at the aquifer boundary. Therefore, the total heat loss over a time step is

$$q_L^{n+1} = q_L^n + \alpha \delta T \Delta t \quad (B-11)$$

where q_L^n is the heat loss with no change in boundary temperature plus the heat loss due to a change in temperature $\alpha\delta T\Delta t$. The constant temperature component (q_L^n) is determined by Fourier's law, written in finite difference form as

$$q_L^n = (K_2^* (T_a - T_1(1))A)\Delta t \quad (B-12)$$

where T_a and $T_1(1)$ are the aquifer and first overburden node temperatures, and A is the area perpendicular to the heat flux path. The additional heat loss due to the change in temperature δT is approximated by

$$\alpha\delta T\Delta t = \left[\frac{K_{ob}}{\Delta z_2^*} (1.0 - T_2(1)) A + \frac{(\rho C_p)_{ob} (\Delta z_1) A}{\Delta t} \right] \delta T\Delta t \quad (B-13)$$

The first set of variables on the left-hand side represents Fourier's law based on the gradient determined by boundary conditions from equation (B-10), and the second set of variables represents the rate of change of storage at the boundary overburden block (shaded region in Figure B-1).

After the time-step (at $t = t^{n+1}$), when δT is known, the temperature profile is updated by assuming boundary conditions of

$$T_3(0,t) = \delta T$$

$$T_3(h,t) = 0.0 \quad (B-14)$$

operating on equation (B-2) and summing the temperature results to the old temperature profile. This is conducted in subprogram [PRINT2] before the printout of overburden temperatures.

WELLBORE HEAT TRANSMISSION

The derivation presented in this section is based on Ramey (1962) and Carslaw and Jaeger (1959, p. 261). The solution permits the estimation of the temperature of fluids in a wellbore tubing as a function of depth and time. Basic assumptions are (a) radial energy flows by conduction, (b) heat flow in the wellbore is rapid compared to heat flow in the formation (heat losses taken as steady state leaving the wellbore and unsteady state in the surrounding rock) and (c) thermal and fluid properties are constant over the increment Δz shown in Figure B-2. The variables q_w and T_o are the mass flow rate and fluid temperature entering the well. The wellbore model calculations proceed over a series of user specified depth increments involving a simultaneous solution of the mechanical and total energy equations. After a series of increments (Δz_1 in length), the average temperature of the fluid is T_1 , and the temperature outside the casing is T_2 . The initial temperature of the rock is T_∞ .

A steady state energy balance across the increment dz (z positive downward) is described by the total energy equation of the form

$$\begin{array}{ccccc} dH & - & \frac{gdz}{g_c J} & = & dQ_H & (B-15) \\ \text{(Change in} & & \text{(Change in} & & \text{(Change in} & \\ \text{Enthalpy)} & & \text{Potential Energy)} & & \text{Energy in Fluid)} \end{array}$$

where incompressible flow is assumed. Change in enthalpy in the increment downward is

$$dH = dU + \frac{d(PV)}{J} = C_p dT + \frac{V dp}{J} \quad (B-16)$$

where V is given as specific volume ($d(\text{ft}^3/\text{lbm})$). If flowing friction losses are ignored over the increment dz , the increase in enthalpy in the flow downhole $\approx$ loss in potential energy. For flow uphole, the loss in enthalpy due to decrease in pressure $\approx$ increase in potential energy, hence the total energy equation becomes

$$C_p dT \approx dQ_H \quad (B-17)$$

Assuming no phase change, the steady state heat loss by the fluid is represented by

$$dq_H = -q_w C_p dT_1 = 2\pi r_1 K_H (T_1 - T_2) dz \quad (B-18)$$

where K_H represents the overall heat transfer coefficient through the wellbore casing.

Heat transfer in the surrounding rocks is envisioned as a problem where unsteady heat transfer from a continuous line source takes place in the radial direction in an infinite media. The governing equation and initial and boundary conditions are

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} = \frac{(\rho C_p)_m}{K_m b} \frac{\partial T}{\partial t}$$

$$T = T_\infty \quad t = 0$$

$$T \rightarrow T_\infty \quad r \rightarrow \infty$$

$$\lim_{r \rightarrow 0} \left(r \frac{\partial T}{\partial r} \right) = \frac{q_H}{2\pi K_m b}$$

Figure B-2. Diagram of a wellbore.

where b = thickness of increment Δz , and K_m is given by equation (6-4).

The solution by Carslaw and Jaeger (1959) is

$$T_2 - T_\infty = \frac{-q_H}{4\pi K_m b} \int_{r_2}^{\infty} \frac{e^{-x}}{r^2 (\rho C_p)_m} \frac{dx}{4K_m b t}$$

or when approximated

$$T_2 - T_\infty \approx \frac{q_H}{2\pi K_m b} \left(-0.29 - \ln\left(\frac{r_2}{2\sqrt{\alpha t}}\right) \right)$$

where $\alpha = K_m / (\rho C_p)_m$, [TDIS]. This means

$$dq_H = \frac{2\pi K_m (T_2 - T_\infty) dz}{f(t)} \quad (B-19)$$

where

$$f(t) = \left[-0.29 - \ln\left(\frac{r_2}{2\sqrt{\alpha t}}\right) \right].$$

Equation (B-19) is most accurate when t is large.

Equation (B-18) is rearranged to give

$$\frac{dT_1}{dz} + \frac{2\pi r_1 K_H}{q_w C_p} (T_1 - T_2) = 0. \quad (B-20)$$

Substituting the right hand side of equation (B-18) into the left side of equation (B-19) gives

$$T_2 = \frac{r_1 K_H T_1 + \frac{K_m}{f(t)} T_\infty}{\left[\frac{K_m}{f(t)} + r_1 K_H \right]} \quad (B-21)$$

Substituting equation (B-20) into equation (B-21) results in equation 17 in

Ramey (1962):

$$\frac{dT_1}{dz} + \frac{T_1 - T_\infty}{\frac{q_w C_p (K_m + r_1 f(t) K_H)}{2\pi r_1 K_H K_m}} = 0$$

or

$$-dT_1 = \frac{T_1 - T_\infty}{\left[\frac{q_w C (K_m + r_1 f(t) K_H)}{2\pi r_1 K_H K_m} \right]} dz. \quad (B-22)$$

The heat loss out of the wellbore as defined by the energy balance given by equation (B-17) becomes

$$-dQ_H = \frac{(T_1 - T_\infty) dz}{\left[\frac{q_w (K_m - r_1 f(t) K_H)}{2\pi r_1 K_H K_m} \right]} \quad (B-23)$$

In the wellbore model, $f(t)$ is evaluated based on cumulative time since the beginning of simulation. Therefore, the best estimate of wellbore heat loss is obtained when the flow rate and temperature in the wellbore are constant for long periods of time. Verification of this heat loss model is given by Ramey (1962).

APPENDIX C

BOUNDARY CONDITIONS RELATED PARAMETERS

INTRODUCTION

This section consists of a detailed explanation of hydraulic boundary conditions. A number of input parameters need further explanation to a reader who is not familiar with some of the boundary condition developments in the petroleum reservoir engineering field. Much of this section is a duplication and elaboration of Appendix B of part one of the INTERCOMP documentation (1976).

The first section deals with the input parameters in the source allocation subprogram, [PROD]. A number of the inputs to the code require further attention. In reading this section, one should remember that allocations based on grid block pressure data from the previous time step are used to compute bottom-hole pressure. Therefore, fluid allocation between the layers during the first time step is always based on mobilities (defined later in this discussion). The final pressure after computing δp at the end of the present time step is updated by adding δp to the value computed in the previous time step. For example,

$$[WHP]^{n+1} = [WHP]^n + \delta P$$

for wellhead pressure ($p_{wh} = [WHP]$).

WELLBORE DATA

The pressure gradient near the source is generally large; hence, the nearest grid block pressure is usually not representative of the wellbore pressure. This phenomenon is shown diagrammatically in Figure C-1 for a production well. The large pressure gradient makes it difficult to determine the pressure in the wellbore without refining the grid size to a sufficiently small size so that the additional pressure drop between the first node and the wellbore becomes negligible. The additional pressure drop is computed by assuming steady flow between the first node and the wellbore with

$$Q = \frac{2\pi r k \Sigma z_k}{\mu} \frac{\Delta p}{\Delta r} = \frac{2\pi k \Sigma z_k}{r_1 \mu \ln\left(\frac{r_1}{r_w}\right)} (p_w - p_1) = \frac{WI^*}{\mu} \Delta p \quad (C-1)$$

for radial flow where WI^* is the well index used by the program. The input data require a well index value which is related to WI^* by

$$WI^* = WI \left(\frac{\mu g_c}{\rho g} \right) \quad (C-2)$$

where

$$WI = \frac{2\pi K \Sigma \Delta z_k}{r_1 \ln\left(\frac{r_1}{r_w}\right)} \quad d(\text{ft}^2/\text{day}) \quad (C-3)$$

in which K is the effective hydraulic conductivity in ft/day. The value of K is representative of the hydraulic conductivity for the entire length of the well screen (Σz_k), including the effects of reservoir damage around the well (skin effects). If the value of K is variable from layer to layer, one may evaluate the $K \Sigma z_k$ term by $\Sigma K_k \Delta z_k$, where K_k is the hydraulic conductivity for each layer of thickness Δz_k .

Figure C-1. Schematic of a wellbore in radial coordinates.

For example, using the following data,

$$\mu = .46 \text{ cp}$$

$$r_w = .375 \text{ ft}$$

$$r_1 = 2.00 \text{ ft}$$

$$K = .0179 \text{ ft/day (3.00 millidarcy (3.0 md))}$$

$$\Sigma z_k = 100 \text{ ft}$$

$$\rho = 62.4 \text{ lbm/ft}^3$$

$$WI^* = \frac{2\pi(3.0\text{md})(100\text{ft})}{\ln\left(\frac{2.0}{.375}\right)} * \frac{.00632\text{ft}^2\text{cp}}{\text{psi-day md}}$$

$$WI^* = 7.12 \frac{\text{ft}^3\text{cp}}{\text{psi-day}}$$

Therefore, if $Q = 600 \text{ ft}^3/\text{day}$, the additional pressure drop between the first block and the wellbore is

$$\Delta P = 600 \frac{\text{ft}^3}{\text{day}} \frac{.46\text{cp psi-day}}{7.12 \text{ ft}^3\text{cp}} = 39 \text{ psi}$$

or the pressure at the edge of the wellbore is 39 psi lower than the first grid block pressure. The input well index is not the same as WI^* . The input well index is

$$WI = \frac{2\pi(.0179\text{ft/day})(100\text{ft})}{\ln\left(\frac{2.0}{.375}\right)} = 6.72\text{ft}^2/\text{day}.$$

Similarly, for cartesian coordinates, INTERCOMP recommends

$$WI = 2\pi K \Sigma \Delta z_k \left(\frac{\bar{r} - r_w}{r_w} \right) \left[\frac{1}{1 - \frac{\bar{r}}{r_w} (1 - \ln(\frac{\bar{r}}{r_w}))} \right] \quad (C-4)$$

where

$$\bar{r} = \sqrt{\Delta x_i \cdot \Delta y_j} / \pi$$

Here, the well index estimates the additional pressure drop between the grid block pressure and bottom-hole pressure of the same grid block. If the well is used for observation only, the value of WI is irrelevant, because there is no additional pressure drop between the grid block and the well.

WELLBORE MODEL SPECIFICATION OPTIONS

The well model consists of two generalized modes of operation. One group of well options fall under the category of specification of bottom-hole conditions [ISURF = 0] and specification of surface conditions [ISURF = 1]. In the former specification, hydraulic pressure losses in the wellbore and heat energy losses to the rocks surrounding the wellbore are not calculated. Under each of the two modes, there are a number of options. The following options are available if the bottom-hole specifications apply [ISURF = 0].

1. Injection (or production) rate is specified and allocated between different layers based on layer mobilities alone [IINDW1 = 1]. This means of allocation is always called by default on the first time step [ITIME = 1]. The model computes a bottom-hole pressure [FPW] in order to achieve the specified flow rate (lbm/day). Enthalpy of the injection fluid is computed from the specified injection temperature [TINJ] and bottom-hole pressure [FPW]. In a production well, the grid block enthalpy [EH] is used to determine rate of energy produced. The concentration of solute injected is [CINJ], and the rate of solute produced is computed from grid block concentration [SW]. For a production well, the values of specified [TINJ] and [CINJ] for injection are ignored; instead, new values are substituted into [TINJ] and [CINJ] based on grid block values. The production fluid temperature [TINJ] is computed from production enthalpy [HINJ] which is computed as follows:

$$H_{i,j} = \frac{\sum_k (Q_{w,i,j,k} H_{i,j,k})}{\sum_k Q_{w,i,j,k}} \quad (C-5)$$

Similarly the production solute concentration is

$$C_{i,j} = \frac{\sum_k (Q_{wi,j,k} C_{i,j,k})}{\sum_k Q_{wi,j,k}} \quad (C-6)$$

where $H_{i,j,k} = [EH]$ and $C_{i,j,k} = [SW]$ are grid block enthalpy and concentration, respectively. The $Q_{wi,j,k} = [QW]$ is the allocated mass flow rate. The temperature is evaluated from enthalpy in equation (C-5) assuming bottom-hole pressure [FPW]. The value of [FPW] or bottom-hole pressure is determined by the method described in the next section; however, if the user decides to use [WI] = 0.0, [FPW] will be assigned zero, or the previous value of well pressure. The user should use an estimate of [WI] if a heat transfer problem is being solved.

The definition of layer mobility is

$$M_{i,j,k} = \left(\frac{k_\ell}{\mu} \right)_{i,j,k} WI_{i,j}^* \quad (C-7)$$

where $K_\ell = [KHL]$ is a user-defined fractional allocation factor usually proportional to the layer hydraulic conductivity times the layer thickness. Therefore, the flow rate per layer is

$$Q_{i,j,k} = \frac{M_{i,j,k}}{\sum_k M_{i,j,k}} Q_{i,j} \quad (C-8)$$

where $Q_{i,j} = [Q]$ is the total flow rate (d(ft³/day)) at well (i,j) and $Q_{i,j,k}$ is the flow rate in the given layer. In actual practice, the program uses mass flux [QW] = d(lbm/day) which is determined by

$$Q_{wi,j,k} = \frac{M_{i,j,k}^*}{\sum_k M_{i,j,k}^*} Q_{wi,j} \quad (C-9)$$

where $Q_{wi,j,k} = [QW]$, and $Q_{wi,j} = [QWT]$, and mobilities are evaluated by

$$[MOBT] = M_{i,j,k}^* = \left(\frac{k_\ell \rho g}{\mu g_c} \right)_{i,j,k} WI_{i,j}^* \quad (C-10)$$

If flow is allocated by mobilities only, the value of [WI] is irrelevant since the value of WI cancels in the computation in equation (C-9).

2. Injection (or production) rate is specified and allocated between different layers by layer mobility times pressure drop between the calculated bottom-hole pressure and grid block pressure [IINDW1] = 2. The injection rate into each layer is

$$Q_{w,i,j,k} = [p_{bh} - p_{i,j,k} + \left(\frac{\rho g}{g_c}\right)_w (h_{i,j,k} - h_{i,j,1})] M_{i,j,k}^* \quad (C-11)$$

where h is the elevation, and $k = 1$ refers to the top grid block elevation open to the well screen. Equation (C-11) is summed over each layer (k) to evaluate the bottom-hole pressure, p_{bh} . The resultant equation is

$$p_{bh} = \frac{Q_{w,i,j}}{\sum_k M_{i,j,k}^*} + \frac{\sum_k [p_{i,j,k} - \left(\frac{\rho g}{g_c}\right)_w (h_{i,j,k} - h_{i,j,1})] M_{i,j,k}^*}{\sum_k M_{i,j,k}^*} \quad (C-12)$$

The bottom-hole pressure p_{bh} is evaluated at the top of the well screen opening; hence, the layer pressures are corrected to elevation $h_{i,j,1}$. The value $Q_{w,i,j}$ is the mass flow rate computed from specified volumetric flow rate $Q_{i,j}$ by

$$Q_{i,j} \rho = Q_{w,i,j} \quad (C-13)$$

Injection enthalpy is calculated from the injection temperature [TINJ] and the bottom-hole pressure from equation (C-12). Injection solute concentration is [CINJ]. Production enthalpy and concentration are computed by equations (C-5) and (C-6).

Equation (C-12) is used with option [IINDW1] = 1 for estimating bottom-hole pressure when the well index is not entered as zero. Bottom-hole pressure is used in computing injection enthalpy and not in allocating fluid in option (1).

The flow rate per layer is

$$Q_{w,i,j,k} = M_{i,j,k}^* [p_{i,j,k} - p_{bh} - \left(\frac{\rho g}{g_c}\right)_w (h_{i,j,k} - h_{i,j,1})] \quad (C-14)$$

where $Q_w = [QW]$ in d(lbm/day).

3. Specified rate is allocated like option (2), except that the rate is adjusted by a semi-implicit formulation to improve the computational stability when $[IINDW1] = -2$. The rate in each layer is computed by

$$Q_{w,i,j,k}^{n+1} = Q_{w,i,j,k}^n + \frac{dQ_w}{dp} \delta p_{i,j,k} \quad (C-15)$$

where $Q_{w,i,j,k}^n$ is the explicit rate of injection determined by equation (C-14) at the previous time step and $\delta p_{i,j,k}$, [DP] is the change in pressure in the adjoining grid block (radial coordinates) over a time step. The implicit term of change of flow rate with respect to p is determined as

$$[QWP] = \frac{dQ_w}{dp} = M_{i,j,k}^* \quad (C-16)$$

which is included as part of the diagonals in the coefficient matrix ([C]) in equation (2-38).

For an injection well, the grid block pressure may increase during a time step, and the total rate of injection may drop. To prevent this problem, an iterative procedure has been set up in subprogram [ITER] to increase the explicit allocation so the specified rate is achieved implicitly. The flow rates are updated after solving for δp in subprogram [PRINT2] and are tabulated in the recurrent printouts of flow rates.

Injection and production enthalpy and concentration are computed like option 2.

4. Both injection (or production) rate $[Q]$ and bottom-hole pressure [BHP] are specified. This option chooses the limiting condition in such a way that the specified rate or pressure will be the governing factor dependent upon not exceeding the other specified value. The flow allocation between different layers is on the basis of mobilities and pressure drop between the wellbore and grid block, $[IINDW1] = 3$, like option (2). The bottom-hole pressure necessary to obtain the specified flow rate (injection or production) is computed and compared to specified bottom-hole pressure. For an injection well, if the calculated bottom-hole pressure is greater than specified, then the flow rate achieved is less than the specified flow rate. If the reverse is true, then the specified flow rate is achieved. If the calculated bottom-hole pressure is less than the specified in a production well, the flow rate achieved by the model is less than specified.

5. Both injection (or production) rate $[Q]$ and bottom-hole pressure $[BHP]$ are specified, like option (4), except the flow allocation between different layers is like option (3) using the semi-implicit formulation, $[IINDW1] = -3$.

When surface conditions are specified, $[ISURF] = 1$, the wellbore model must be solved along with the reservoir model. This may require an iterative procedure between the wellbore and reservoir model results from the previous time step. The wellbore and well flow allocation options include (a) a specified flow rate $[IINDW1] = 1, 2, \text{ or } -2$, or (b) a specification of flow rate and surface pressure where the governing factor is chosen so as not to exceed the other specified value $[IINDW1] = 3 \text{ or } -3$. Fluid allocation in the individual layers are conducted in the same manner as options (1) to (5). Each surface option specified is discussed in the following section.

6. Injection (or production) rate is specified, $[IINDW1] = 1, 2 \text{ or } -2$. For an injection well, the surface temperature $[TINJ]$ is specified. Surface pressure cannot be specified because the bottom-hole pressure, $p_{bh} = [FWP]$, is determined from specified flow rate and grid block pressure $p_g = [P]$, by equation (C-12). Wellbore calculations of heat loss and hydraulic head loss proceed from the surface to the aquifer by first assuming a value of surface pressure and calculating bottom-hole pressure, $P_{cal} = [PBOT]$, by the wellbore model. This procedure is repeated with a new surface pressure until the bottom-hole pressure by the wellbore model is within toleration limits of the reservoir-determined bottom-hole pressure, $p_{bh} = [FWP]$, to inject the specified flow rate, and the final surface pressure is assigned $[WHP]$, or well-head pressure.

Toleration limits are related to the input data as follows:

$$[ERRDP = \text{ABS}(PBOT-FWP)]$$

$[IF(ERRDP.LE.TOLDP)]$ iteration tolerance is satisfied.

The variables $[PBOT]$ and $[FWP]$ are calculated bottom-hole pressure by wellbore model, and bottom-hole pressure based on grid block pressure calculated from specified flow rate, respectively. The variable $[TOLDP]$ is the input tolerance for pressure $d(\text{psi})$. Well index should be specified for all allocation options to make use of equation (C-12) to accurately compute bottom-hole pressure from grid block pressure.

For a production well, the bottom-hole pressure necessary to produce the specified rate is calculated directly from reservoir grid block

pressure, and wellbore model calculations proceed from the well bottom to the top of the production well so there is no need for iteration to compute surface pressure [WHP] from bottom-hole pressure.

Specified flow rates and specified surface pressure are handled together in one option: [ISURF] = 1 and [IINDW1] = 3 or -3.

7. This option considers the case where both surface pressure [THP], and injection or production rates are specified by the user ([ISURF] = 1 and [IINDW1] = 3 or -3). The solution method takes the lower value of the flow rate calculated from the surface pressure or a specified rate. The solution begins with the specified rate information, and calculates the corresponding surface pressure. For an injection well, if this surface pressure is higher than the specified pressure [THP], a new flow rate is calculated based on the limitation of a specified top-hole pressure [THP]. The specified flow rate is allocated when the calculated surface pressure is lower than the specified surface pressure.

For an injection well the solution begins by using equation (C-13) and (C-12) to obtain a calculated bottom-hole pressure [FWP]. The estimated flow rate per layer is obtained by equation (C-14). The program estimates a top-hole pressure [PREF] by subtracting the static pressure head based on the length of the wellbore from [FWP]. The wellbore model uses the estimated top-hole pressure [PREF], injection temperature [TINJ] and flow rate to obtain a second bottom-hole pressure [PBOT]. The two bottom-hole pressures are compared for tolerance as shown in option (6). If the tolerance is not satisfied, [PREF] is updated by summing [FWP - PBOT] to [PREF] to obtain a new estimated top-hole pressure. This procedure continues until the difference [FWP - PBOT] is within a given tolerance as shown in option 6. When the tolerance is satisfied the estimated top-hole pressure [PREF] is compared to the specified top-hole pressure [THP], and if [PREF] is less than or equal to [THP], solution has converged, and the specified flow rate is used in injection allocation. Otherwise an iterative procedure is set-up to determine the new flow rates based on [THP].

The basic procedure for calculating the flow rates controlled by the specified top-hole pressure [THP] begins as follows. The estimated bottom-hole pressure is $[BHPS] = [THP] + \rho g[X]/g_c$ where [X] is the length of the wellbore. The solution procedure updates the bottom-hole pressure by setting [FWP] = [BHPS] and solves equation (C-14) to determine allocated flow rate. An estimated top-hole pressure [PREF] is determined by subtracting the static hydraulic head from [FWP], and the estimated top-hole pressure [PREF], injection temperature [TINJ] and flow rate are used in the wellbore model to determine a new bottom-hole pressure [PBOT]. The bottom-hole pressures are checked for convergence by the method given in option (6). If convergence is satisfied, solution is completed, otherwise the change in flow rate over an iteration is checked by

$$[ERR1 = \text{ABS}(QWDEL - QWT)]$$

[IF (ERR1 .LT. TOLX)] toleration is satisfied for injection rates.

The above terms are defined as follows: [QWDEL] = calculated injection rate for a well at the previous iteration, [QWT] = the calculated injection rate at the present iteration, and [TOLX] is the user-specified tolerance factor. In addition if tolerance has not been satisfied the following is checked

[ERR = ABS (PBOT - FWP)/FWP]
[IF(ERR .LE. TOLX)] tolerance is satisfied.

If none of the above tolerance conditions are satisfied, and [PBOT] is greater than or equal to the grid-block pressure, the following is used to estimate a new bottom-hole pressure ([BHPS]):

$$[BHPS = (FWP + DAMPX PBOT)/(1 + DAMPX)]$$

where [DAMPX] is a user-specified damping factor used to estimate a new bottom-hole pressure. If [PBOT] is less than the grid-block pressure the new bottom-hole pressure is

$$[BHPS = 0.5*(FWP + PFW)]$$

where [PFW] is the grid-block pressure, determined at the previous time step. The maximum number of iterations are limited by a user specified maximum, [NITQ]. Iterations continue until one of the above tolerances is satisfied, or the number of iterations exceed the user-specified maximum of [NITQ]. The above is one example of each usage of user specified [DAMPX], [TOLX] and [TOLDP] in the subprogram [PROD].

A similar procedure is used for a production well. The program assumes a bottom-hole pressure computed by equations (C-13) and (C-12). An allocated flow rate is computed by equation (C-14) based on grid-block pressure, and assumes bottom-hole pressure. The wellbore model proceeds from the bottom-hole using the computed flow rate, bottom-hole pressure and temperature to compute a surface pressure. The calculated surface pressure is compared with the specified surface pressure. If the calculated pressure [PTOP] is greater than or equal to the specified surface pressure [THP], convergence is achieved and specified flow rates are used. If convergence is not achieved, the program begins an iterative procedure to compute a bottom-hole pressure [BHPS] such that the calculated flow rates and the bottom-hole pressure combination result in a corresponding calculated top-hole pressure [PTOP] that is within tolerance of the specified top-hole pressure [THP] like that shown in option (6). If pressure tolerance is not satisfied the program checks whether flow rates have changed significantly over an iteration. If flow rates have not changed by much, the solution has converged. If convergence has not been achieved relative pressure tolerance is checked, and if tolerance is not satisfied a new value of [BHPS] = [FWP] is computed and the iteration repeats until either convergence is satisfied or the maximum number of iterations, [NITQ] has been exceeded.

A summary listing of well options are listed in Table C-1. One should note that the use of the wellbore model assumes no interference from other sources of thermal energy. This assumption is not true near the base of the wellbore because of overburden conduction and energy transfer in the reservoir. If the length of the wellbore is short compared to the region of reservoir thermal influence penetrated by the wellbore, the prediction of heat loss or gain by the wellbore model is expected to be inaccurate (see Figure C-1).

Table C-1. Summary of Well Specification Options¹

Option No.	Specification	Quantities Specified	Allocation Basis	Rate	Limiting Criterion
1	Bottom-hole	Rate	Mobilities	Explicit	None
2	Bottom-hole	Rate	Mobilities and pressure drop	Explicit	None
3	Bottom-hole	Rate	Mobilities and pressure drop	Semi-implicit	None
4	Bottom-hole	Rate and bottom-hole pressure	Mobilities and pressure drop	Explicit	[Calculated or specified bottom-hole pressure, whichever is limiting]
5	Bottom-hole	Rate and bottom-hole pressure	Mobilities and pressure drop	Semi-implicit	
6	Surface	Rate	Mobilities	Explicit	None
7	Surface	Rate	Mobilities and pressure drop	Explicit	None
8	Surface	Rate	Mobilities and pressure drop	Semi-implicit	None
9	Surface	Rate and surface pressure	Mobilities and pressure drop	Explicit	[Calculated or specified surface pressure, whichever is limiting]
10	Surface	Rate and surface pressure	Mobilities and pressure drop	Semi-implicit	

¹Adapted from INTERCOMP, 1976, Table B-1, Part I)

AQUIFER INFLUENCE FUNCTIONS

Aquifer influence functions are options of hydraulic boundary conditions that allow the user to simulate an infinite or finitely large aquifer without the expense of a large numerical finite difference grid. Aquifer influence functions are not needed when the numerical grid system is not subjected to changes in pressure, temperature, and concentration along the exterior boundaries during the time of interest. No aquifer influence functions at the grid block boundary translates to no fluid influx or efflux or to an impermeable boundary. For most problems, the compressibility of the fluid and matrix are small; therefore, the pressure rapidly effects travel. Over a large enough period aquifer influence (fluid influx or efflux) calculations are required to adequately simulate a large or infinite aquifer.

The INTERCOMP code offers three aquifer influence options. The Carter-Tracy method (Carter and Tracy, 1960) gives the best results for an infinite aquifer representation. The pot aquifer representation is the simplest and is useful for history matching; the steady state method is the best choice when pressure is maintained along the external boundary for natural flow in the aquifer. Each of these methods and input data are discussed in the following section.

An estimate of the numerical mesh size required to avoid using aquifer influence functions is

$$r_e = 2\sqrt{kt^*/(39\mu\phi c_t)} \quad (C-17)$$

where

r_e = radius, (ft)

k = permeability, (md) ($1 \text{ md} \approx 2.7 \times 10^{-3} \text{ ft/day for water } 70^\circ\text{C}$)

ϕ = porosity

c_t = total compressibility $\approx c_R + c_w$, (1/psi)

μ = viscosity, (cp) and t^* = time span of interest, (days).

A grid that has an effective radius of r_e , given by equation (C-17), acts as an infinite aquifer for t^* days.

Carter-Tracy

This influx boundary condition assumes a scenario given in Figure C-1, where the numerical grid ends at external radius r_e . The method assumes that the aquifer is homogeneous. This condition may not always exist, so a representative aquifer parameter may be used. The isotropic assumption does not enter because influx or efflux is assumed to be in one direction only; hence, in summary, the Carter-Tracy (1960) method allows a homogeneous infinite aquifer to be simulated through the use of a finite region based on an approximation to the superposition method of Van Everdingen and Hurst (1949). The development and tables of solutions are given in the latter and the approximation is given in the former reference.

According to Carter and Tracy (1960, equation 8) the cumulative influx through a circular aquifer of radius r_e is

$$d(\text{ft}^3) \quad W^{n+1} = W^n + \frac{B\Delta p^{n+1} - W^n p_d^{n+1}}{p_d^{n+1} - t_d^n p_d^{n+1}} (t_d^{n+1} - t_d^n). \quad (\text{C-18})$$

Therefore, the quantity of water influx over time t^n to t^{n+1} is

$$e_w^{n+1} = \left(\frac{dW}{dt}\right)^{n+1} = \frac{W^{n+1} - W^n}{t^{n+1} - t^n}$$

$$d(\text{ft}^3/\text{day}) e_w^{n+1} = k_t \frac{B(p^i - p^n) - B(p^{n+1} - p^n) - w^n p_d'^{n+1}}{p_d^{n+1} - t_d^n p_d'^{n+1}} \quad (C-19)$$

where

$$B = 2\pi b \phi c_t (r_e)^2 s$$

s = fraction of circle covered by circular aquifer [VAB]

b = thickness of aquifer (ft)

p^i = initial pressure in grid block (psi)

p^n = grid block pressure at t^n (psi)

w^n = cumulative water influx at time t^n (ft³)

$p_d' = dp_d/dt_d$ (dimensionless)

$k_t = t_d/t = k/(\mu \phi c_t r_e^2)$ (1/day)

$t_d = (kt)/(\mu \phi c_t r_e^2)$ = dimensionless time

k = effective permeability at the periphery

$p_d = p_d(t_d)$ = dimensionless pressure from "terminal rate case" from Van Everdingen and Hurst.

The basic form of equation (C-19) is

$$e_w = a - b \phi p \quad (C-20)$$

where

$$a = \frac{B(p^i - p^n) - w^n p_d'^{n+1}}{p_d^{n+1} - t_d^n p_d'^{n+1}} k_t \quad [\text{AAQ}]$$

$$b = \frac{B k_t}{p_d^{n+1} - t_d^n p_d'^{n+1}} \quad [\text{BAQ}]$$

and

$$\delta p = p^{n+1} + p^n$$

evaluated at the periphery grid block. The model includes the data for $P(t_d) = P_d$ vs. t_d for an infinite aquifer. For a finite aquifer, the values of $P(t_d)$ vs. t_d have to be read in from Table C-2. Ratios of r_L/r_e refer to ratios of true aquifer boundary, r_L , to the boundary used by the model and r_e in Table C-2.

In the above discussion, equations (C-19) and (C-20) refer to efflux rates (or influx) to the entire aquifer; however, pressures are determined at the individual grid blocks, which may be arranged in Cartesian coordinates rather than radial coordinates. The following section discusses the use of the Carter-Tracy method with Cartesian coordinate block arrangement.

Consider a general case where an infinite aquifer is to be simulated with $N \times N$ grid blocks in the x and y direction, respectively, and with uniform grid spacing $\Delta x = \Delta y = \text{constant}$. The equivalent radius is

$$\pi r_c^2 \approx (N-1)\Delta x(N-1)\Delta y.$$

The rectangular grid boundary is replaced by an equivalent circle. The water efflux at each boundary block (i,j) column of $[NZ]$ blocks is a site specific form of equation (C-20):

$$e_{w,i,j} = a_{ij} - b_{ij} \delta p_{ij} \quad (C-21)$$

where a_{ij} and b_{ij} are made site specific by specifying

$$B_{ij} = 2\pi b\phi c_t r_e^2 S_{ij} \quad (C-22)$$

where s_{ij} is the fraction of a circle edge assigned to the edge grid block column consisting of [NZ] blocks at areal position (i,j). For this problem, the total perimeter is

$$L = 4(N - 1)\Delta x \quad (C-23)$$

and s_{ij} is $\Delta x_i/L$ for all the grid blocks with the exception of the corner blocks where s_{ij} is $\Delta x_i/L$.

In more general cases, the equivalent radius is

$$r_e \approx \sqrt{L_x L_y / \pi} \quad (C-24)$$

where L_x and L_y are lengths along the x-direction and y-direction of the rectangular grid. The grid should be kept as square as possible in order to estimate the circular reservoir influence functions. The total perimeter is

$$L = 2 \sum_{j=1}^{N_y} \Delta y_j + 2 \sum_{i=1}^{N_x} \Delta x_i \quad (C-25)$$

where N_x and N_y are the number of grid blocks in x and y-directions, and Δx_i and Δy_j are the grid increments. The value of s_{ij} in (C-22) is now $\Delta x_i/L$ and $\Delta y_j/L$ for the x- and y-direction edges, respectively, and $(\Delta x_i + \Delta y_j)/L$ for the four corner blocks. Smaller and larger values of $s_{i,j}$ [VAB] may be used for certain edge blocks to represent aquifer heterogeneity along the periphery. The physical meaning of this variation is not clear and should be used with caution. The variable $s_{i,j}$ in its most general form is $s_{i,j,k}$ where the latter represents the fraction of the aquifer perimeter and depth open to the aquifer influence functions.

Table C-2. Carter-Tracy Functions for Limited Reservoirs¹

$r_L/r_e = 2$		$r_L/r_e = 3$		$r_L/r_e = 5$		$r_L/r_e = 10$	
Dimensionless Time (t_d)	Pressure Change (P_d)	Dimensionless Time (t_d)	Pressure Change (P_d)	Dimensionless Time (t_d)	Pressure Change (P_d)	Dimensionless Time (t_d)	Pressure Change (P_d)
0.22	0.443	0.50	0.627	3.0	1.167	12.0	1.732
0.24	0.459	0.54	0.636	3.2	1.192	13.0	1.768
0.26	0.476	0.56	0.645	3.4	1.215	14.0	1.801
0.28	0.492	0.60	0.662	3.6	1.238	15.0	1.832
0.30	0.507	0.65	0.683	3.8	1.259	16.0	1.862
0.32	0.522	0.70	0.703	4.0	1.281	17.0	1.890
0.34	0.536	0.75	0.721	4.2	1.301	18.0	1.917
0.36	0.551	0.80	0.740	4.4	1.321	19.0	1.943
0.38	0.565	0.85	0.758	4.6	1.340	20.0	1.968
0.40	0.575	0.90	0.776	4.8	1.360	22.0	2.017
0.42	0.593	0.95	0.791	5.0	1.378	24.0	2.063
0.44	0.607	1.00	0.806	5.5	1.424	26.0	2.108
0.46	0.621	1.20	0.855	6.0	1.469	28.0	2.151
0.48	0.634	1.40	0.920	6.5	1.513	30.0	2.194
0.50	0.648	1.60	0.973	7.0	1.556	32.0	2.236
0.60	0.715	2.00	1.076	7.5	1.598	34.0	2.278
0.70	0.782	3.00	1.328	8.0	1.641	36.0	2.319
0.80	0.849	4.00	1.578	9.0	1.725	38.0	2.360
0.90	0.915	5.00	1.828	10.0	1.808	40.0	2.401
1.00	0.982			11.0	1.892	50.0	2.604
2.00	1.649			12.0	1.975	60.0	2.806
3.00	2.316			13.0	2.059	70.0	3.008
5.00	3.649			14.0	2.142		
				15.0	2.225		

¹Adapted from INTERA, 1979. Additional tabulations of r_L/r_e ratios can be obtained directly from Table III in Van Everdingen and Hurst (1949).

Pot Aquifer

Influx rate is a function of the change in pressure in any peripheral grid block, the compressibility of the aquifer, and the total pore volume of the selected grid block mesh. Similar to the Carter-Tracy method, influx rate during a time step between t^{n+1} and t^n can be expressed as

$$e_w^{n+1} = \left(\frac{dw}{dt}\right)^{n+1} = \frac{w^{n+1} - w^n}{t^{n+1} - t^n} = \frac{\phi_1 (p^n - p^{n+1})}{(t^{n+1} - t^n)} \quad d(ft^3/day) \quad (C-26)$$

where ϕ_1 is the aquifer influx coefficient in ft^3/psi .

To illustrate how the method works, envision an injection well where the pressure in the aquifer increases with time if all the aquifer peripheral boundaries are impermeable. All the fluid injected during a time step n to $n+1$ is retained in the aquifer so

$$Q = V_p c_t \frac{(\bar{p}^{n+1} - \bar{p}^n)}{(t^{n+1} - t^n)} \quad (C-27)$$

or the increase in pressure is

$$(\bar{p}^{n+1} - \bar{p}^n) = \frac{Q(t^{n+1} - t^n)}{c_t V_p} \quad (C-28)$$

where

$$c_t = \phi c_w + (1-\phi) c_R \quad (1/psi)$$

$$V_p = \text{total pore volume of aquifer } (ft^3)$$

$$Q = \text{injection rate } (ft^3/day)$$

$$t = \text{time (days)}$$

$$n = \text{time level}$$

$$\bar{p}^n = \text{average pressure in the aquifer at beginning of time } = t^n.$$

When the efflux rate is equal to the injection rate, the pressure gradient in the aquifer does not change significantly with time, and the increase in pressure in the peripheral grid blocks is nearly the same as the increase in the average pressure. Letting $Q = -e_w^{n+1}$ in equation (C-26) and combining it with equation (C-27), the result is

$$v_1 = v_p^c \quad (C-29)$$

The pressure distribution in a pot aquifer is known as semi-steady state pressure distribution and implies that the periphery pressure may increase gradually without bounds.

Block influx is expressed in a similar manner as the Carter-Tracy boundary efflux method because equation (C-26) represents efflux (or influx) to the entire aquifer. The influx representation for a single block is

$$e_{w_{ij}} = \alpha_{ij} v_1 \frac{(p^n - p^{n+1})}{(t^{n+1} - t^n)} \quad (C-30)$$

where α_{ij} reflects the fraction of the field perimeter represented by the edge grid block column. Like the Carter-Tracy method, α_{ij} can be modified to adjust flow rate for aquifer heterogeneity at the boundary. The value of v_1 can be adjusted to deviate from the definition given in equation (C-29) to better match pressure history if the data are available. Input data require

$$[VAB] = \alpha_{ij} v_1 \quad d(\text{ft}^3/\text{psi})$$

over a region.

Steady-State Aquifer

Schilthuis (1936), proposed the following expression for calculating cumulative water influx into an aquifer:

$$w_{(t)} = \nu_2 \int_0^t (p^i - \bar{p}) dt \quad d(ft^3) \quad (C-31)$$

where ν_2 is the aquifer influx coefficient in $ft^3/day^2/psi$, $\bar{p}$ is the average pressure at the aquifer boundary at time t , and p^i is the initial pressure. The rate of influx between time t^n and t^{n+1} for the aquifer is

$$e_w^{n+1} = \left(\frac{dw}{dt}\right)^{n+1} = \nu_2 (p^i - p^{n+1}) \quad d(ft^3/day). \quad (C-32)$$

When the rate of efflux becomes equal to rate of injection, the pressure distribution in the aquifer represents a steady state condition. The exterior boundary pressure is set equal to initial pressure p^i and p^{n+1} is the average pressure in the edge boundary blocks at the $n+1$ time level. The coefficient ν_2 can be computed by applying Darcy's law at the periphery. For example, consider a circular aquifer with model external radius r_e and radius to the edge block center, r_n (see Figure C-1). At steady-state

$$Q = \frac{2\pi kb}{\mu} \frac{(p^{n+1} - p^i)}{\ln \left(\frac{r_e}{r_n}\right)} \quad (C-33)$$

and since

$$Q = - e_w \quad (C-34)$$

the coefficient $\mathfrak{J}_2$ is obtained by substituting equation (C-33) into equation (C-32) to get

$$v_2 = \frac{-2\pi kb}{\mu \ln\left(\frac{r_e}{r_n}\right)} d(\text{ft}^3/(\text{psi-day})) \quad (\text{C-35})$$

The efflux at an individual block is

$$e_{w_{ij}} = \alpha_{ij} v_2 (p^i - p^{n+1}) \quad (\text{C-36})$$

where α_{ij} is the fraction of the exterior perimeter represented by edge block column (ij). Since efflux rate will never exceed the rate of injection, the pressure in the edge block has an upper bound which can be evaluated by equation (C-33). The input data require

$$[\text{VAB}] = \alpha_{ij} v_2$$

defined for a region.

Test responses of the aquifer influence functions are shown in Figure C-2. Comparisons are made of various aquifer influence options using the same aquifer properties and flow rates. The aquifer influence functions model used an external radius of $r_e = 337$ ft. One model run was tested using $r_e = 2000$ ft with impermeable boundaries for comparison. The variability of the pot aquifer for history matching is demonstrated by using the formula in equation (C-29) and an arbitrary value of $\mathfrak{J}_1 = 10^6$. Note that the pressure in the pot aquifer formulation increases without bounds as suggested in its formulation. The analytical solution is the same as the Theis solution.

Figure C-2. Test of aquifer influence functions, at an observation well located at $r = 45$ ft. (adapted from Figure 10 in INTERCOMP, 1976).

APPENDIX D

USERS INSTRUCTIONS

CHANGES IN THE NOMENCLATURE

The blocking of computer variable VAR denoted by [VAR] is now denoted by VAR. This change is in effect for all text in Appendix D because of the large number of referrals to computer variables.

REDIMENSIONING THE PROGRAM

The use of variables stored in a REAL*8 data format requires a slight change in redimensioning instructions. The fixed common block consists of a section containing REAL*8 variables containing members from BW0 to UWN. Fixed common block members in REAL*4 begin with EHF and end with IDLAST. The partitioned common block begins with GD and ends with G. The GD common contains the REAL*8 arrays, G contains the REAL*4 arrays, and the DUMMY variable assures that GD begins on an even REAL*4 word. The individual member arrays are determined from input data in the MAIN program. The starting position of each member array is stored in IDLX to IDLAST, and GD and G members are passed through as subroutine arguments.

This data storage design was used because the number of arguments passed through any given subroutine is limited to 63 in a Control Data machine. Therefore, some of the variables need to be passed through the fixed size common block. This limitation applies to the following:

Maximum number of wells	20
Number of overburden and underburden layers	7
Number of Carter-Tracy aquifer influence functions,PTD,TTD	50
Number of entries in each of the viscosity and temperature tables	10

For problems that exceed the above limitations the following fixed common block arrays should be redimensioned as follows:

<u>Array Names</u>	<u>Number of Arrays</u>	<u>Dimension as</u>
SC,VCC	2	Number of entries in the concentration-viscosity table.
TR,VISR	2	Number of entries in the temperature-viscosity table for the resident (reservoir) fluid.
TI,VISI	2	Number of entries in the temperature-viscosity table for the injection fluid.
ZT,TD	2	Number of entries in the depth-temperature table.
PTD,TTD	2	Number of aquifer influence functions.
CCOB,COB,DZOB, UOB,UUOB	5	Number of overburden layers.
CCUB,CUB,DZUB, UUB,UUUB	5	Number of underburden layers.
TZOB	1	Number of overburden layers + 1.
TZUB	1	Number of underburden layers + 1.
EE	1	Larger of the number of overburden and underburden layers + 1.
BHP through WI	31	Number of wells.

When increasing the number of overburden or underburden blocks or the number of wells, the following changes must be made in the MAIN program:

Change:

NOBMX = 7 to number of overburden blocks or layers
 NUBMX = 7 to number of underburden blocks or layers.
 NWMAX = 20 to number of wells or layers.

Since the above changes apply to all the subroutines that address the fix common block, nearly every subroutine has to be recompiled.

The storage location of IDLAST should be determined. If the number of the storage location is an odd number, the variable DUMMY is not required in the statement COMMON DUMMY,GD(.),G(.). For most problems only the size of GD and G needs to be changed; hence, only the MAIN program requires recompiling.

This economical method of reallocating storage assumes that all other subprogram parts have been compiled and stored separately as an object deck. The MAIN program is compiled and linked to the other subprograms and stored as a load module for execution. Therefore, in practice, the only limitation on the problem size is the core size of the machine used.

INPUT DATA CARDS

READ M1 (20A4/20A4)

LIST: TITLE

TITLE Two cards of alphanumeric data to serve as a title for this run. Any title up to 160 characters (80 per card) in length may be used.

READ M-2 (8I5)

LIST: NCALL, RSTRT, ISURF, IPDIM, IIPRT, NPLP, NPLT, NPLC

NCALL Control parameter for solving the basic partial differential equations. If you desire to simulate a solution of all three equations, enter zero (0). The pressure equation is always solved. The solutions of the temperature and concentration equations may be bypassed, if desired.

0 - All three equations will be solved.

-2 - The concentration equation will not be solved. The simulated solution will consist of solving a set of two coupled equations of pressure and temperature.

1 - The pressure equation will be solved. The model is simplified to solving one independent partial differential equation.

2 - The temperature equation will not be solved. The model solves two coupled partial differential equations for pressure and solute transport.

RSTRT The number of the time step at which calculations are to resume for a restart run (ITIME in the program output). A restart record from a previous simulation run corresponding to the specified time step must exist on the restart tape mounted on tape unit number 4. An output tape should be available on unit 8.

For a nonrestart run, i.e., a run from initial conditions, enter RSTRT as zero (0).

ISURF Control parameter for wellbore calculations.

- 0 - No wellbore calculations will be performed. This means only well flow rates or bottom-hole pressures may be specified.
- 1 - Wellbore calculations will be performed.

IPDIM Blank common printing key. The total length of the blank common may be printed. This is useful in writing restart records. The length of the blank common is the storage space required on the tape every time a restart record is written.

- 0 - Blank common length is not printed.
- 1 - Blank common length is printed.

IIPRT Transmissibilities printing key. The printing of Darcy velocities, fluid properties, and transmissibilities calculated from conditions in the aquifer at the previous time step are activated by this print key. Print key entered here is effective from the first time step until it is changed in the recurrent data READ R2-11. Print tables activated by this print key are only printed at TCHG (READ R2-10). If this is a restart run, this transmissibility printing key has no meaning.

- 0 - No transmissibility, Darcy velocity, and fluid property output are activated.
- 1 - All transmissibilities, Darcy velocities, and fluid properties calculated at the old time level are printed.
- 2 - Only Darcy velocities calculated at the old time level are printed.

NPLP Control parameter for plotting pressures in wells.

- 1 - Bottom-hole and surface pressures are plotted if wellbore calculations are performed. Only the bottom-hole pressures are plotted if no wellbore calculation are performed. For an observation well, the bottom-hole pressure is the grid block pressure.
- 0 - If no pressure plots are desired.
- 1 - If pressure plots are desired for a previous run, skip READ M-3 through R2-15, and proceed to READ P-1.

NPLT Control parameter for plotting temperatures in the well.

- 1 - For an observation well, the grid block temperature is plotted. For an injection well, the bottom-hole temperature is plotted if wellbore calculations are performed. For a production well, the bottom-hole temperature is always plotted. In

addition, the surface temperature is plotted if the wellbore calculations are performed.

- 0 - If no temperature plots are desired.
- 1 - If temperature plots are desired for a previous run, skip READ M-3 through R2-15, and proceed to READ P-1.

NPLC Control parameter for plotting concentration in the well.

- 1 - The concentration in the well is plotted for observation and production wells only.
- 0 - If no concentration plots are desired.
- 1 - If concentration plots are desired for a previous run, skip READ M-3, through R2-15 and proceed to READ P-1.

NOTE: Proceed to READ P-1 if any of the NPL's are negative. If any NPL's are negative, input data from a previous run must be available on (tape) unit number 12.

READ M-3 (10I5)

These data will be used to dimension the arrays needed in the code. The program is designed to calculate its internal array size. This allows for minimal redimensioning effort throughout remainder of the program.

LIST: NX, NY, NZ, HTG, KOUT, PRT, NABLMX, METHOD, ISZE, NAR

- NX Number of grid cells in the x-direction (greater than or equal to 2).
- NY Number of grid cells in the y-direction (greater than or equal to 1).
- NZ Number of grid cells in the z-direction (greater than or equal to 1).
- HTG Control parameter for input of reservoir description data. If you desire to specify a heterogeneous aquifer, you may enter either HTG = 2 and enter data for each block or series of blocks, or specify a homogeneous linear or radial geometry aquifer and modify the blocks or regions in which heterogeneity is desired.
 - 1 - Homogeneous aquifer, of linear geometry.
 - 2 - Heterogeneous aquifer, where data are read for each grid block or series of blocks. The aquifer configuration is a linear geometry.
 - 3 - Radial geometry aquifer. The aquifer may be heterogeneous in the vertical direction in the form of layers.

KOUT Output control parameter.

- 0 - All program output are activated.
- 1 - All program output except for initial arrays (concentrations, pressures, etc.) are activated.
- 3 - No program output are activated. KOUT is read again in the recurrent data entry READ R2-11. A value of KOUT here of 3 can be used to omit printing of all initialization data as is sometimes desirable in making a sequence of many history matching runs.

PRT Output array orientation control parameter.

- 1 - Print output maps as areal layers (x-y). Block numbers in the x-direction increase from left to right and decrease down the computer page in the y-direction.
- +1 - Print out is similar to the above except the J-block numbers (y-direction) increase down the computer page.
- 2 - Print output maps as vertical sections (x-z).

NABLX This is the maximum number of aquifer influence function blocks. This value is used for dimensioning the aquifer influence function arrays. This number is usually equal to the number of peripheral blocks.

METHOD The control parameter that determines the method of solution used for the current run. The method of solution entered here will be used to dimension the working arrays in the numerical solution sub-routines (direct solution or L2SOR). The method to be used is read again in the recurrent data entry READ R2-2. Since the amount of storage for direct solution is always greater than for L2SOR, you may specify direct solution on the card and may actually use L2SOR, but you may not specify L2SOR on this card and use direct solution later.

- 0,±1 Allocate storage for direct solution. You may specify either direct solution or L2SOR in READ R2-2. The dimension of a working array "A" is printed out at this point. If you specify direct solution again in READ R2-2, the minimum length required for the "A" array will be printed. This length must be smaller than the dimension of array "A". If it is not, you must use the L2SOR method or, enter a new "A" array dimension by NAR.
- ±2 - Allocate storage for L2SOR method. You may not specify direct solution in READ R2-2.

ISZE Control parameter used to stop program after computing the size of the core required for the run.

- 0 - Program will continue after printing common block size.
- 1 - Program will halt after printing common block size. The input data ends at READ M-3.

NAR Storage allocation for working array "A" in direct solution routine GAUS3D.

- 0 - Dimension of "A" array is to be approximated internally. The program will calculate the exact length of "A" later. If the approximate length is less than the exact length, the size of "A" should be entered via NAR if direct solution is desired.
- >0 - Storage dimension for "A" array. If direct solution is desired this number must be greater than or equal to the minimum length required which is printed later in the program.

READ M-4 (F10.0)

NOTE: This card is read only if the run is a restart, i.e. only if the value for RSTRT is non-zero.

LIST: TMCHG

TMCHG Time in days at which the next set of recurrent data is to be read. If TMCHG is less than or equal to the time corresponding to the restart time step number, a set of recurrent data will be read immediately to resume the previous simulation.

NOTE: Proceed to READ R2-1 (recurrent data entry) if RSTRT is non-zero.

READ R1-1 (5E10.0)

LIST: CW, CR, CTW, CPW, CPR

CW Compressibility of the aquifer fluid, $(\text{psi})^{-1}$.

CR Compressibility of rock, $(\text{psi})^{-1}$.

CTW Coefficient of thermal expansion of the aquifer fluid, $(^{\circ}\text{F})^{-1}$.

CPW Fluid heat capacity, $(\text{Btu}/(\text{lbm}-^{\circ}\text{F}))$.

CPR Rock heat capacity per unit volume, $(\text{Btu}/(\text{ft}^3-^{\circ}\text{F}))$.

READ R1-2 (7E10.0)

LIST: UKTX, UKTY, UKTZ, CONV, ALPHL, ALPHT, DMEFF

UKTX Thermal conductivity of the porous medium in the x-direction $(\text{Btu}/\text{ft}-^{\circ}\text{F day} - \text{see CONV})$. The value entered here is a thermal conductivity of the fluid and the solid in the porous medium.

UKTY Thermal conductivity of the porous medium in the y-direction.

UKTZ Thermal conductivity of the porous medium in the z-direction.

CONV Conversion factor for the thermal conductivities. The entered values of the thermal conductivities are multiplied by CONV to obtain Btu/(ft-day-°F) units. If CONV is entered as zero, thermal conductivities should be read in Btu/(ft-day-°F).

ALPHL Longitudinal dispersivity factor, ft.

ALPHT Transverse dispersivity factor, ft.

DMEFF Molecular diffusivity in the porous media, ft²/day.

READ R1-3 (4E10.0)

The fluid densities are entered here at concentration = 0 (natural aquifer fluid) and concentration = 1 (injection fluid). Both the densities should be entered at the same reference temperature and pressure. This information is used to relate concentration to mass of fluid injected or produced.

LIST: PBWR, TBWR, BWRN, BWRI

PBWR Reference pressure at which the densities are to be entered, psi.

TBWR Reference temperature at which the densities are to be entered, °F.

BWRN The density of the natural aquifer fluid (concentration = 0) at PBWR and TBWR, lbm/ft³. Note that densities are entered in pound mass/unit volume.

BWRI The density of the injection fluid (concentration = 1) at PBWR and TBWR, lbm/ft³.

READ R1-4 (I5)

NOTE: If ISURF = 0, omit READ R1-4 and R1-5 and proceed to R1-6.

LIST: NOUT

NOUT Output control parameter for wellbore calculations.

- 0 - No output is activated.
- 1 - Iteration summary (number of outer iterations, flow rate, and the bottom-hole pressure) is printed for each well.
- 2 - The well pressure and temperature (at the surface for an injection well and at the bottom-hole for a production well) and the flow rate are printed every time subroutine WELLB is called.

- 3 - The pressure and temperature in the well are printed over each increment (see DELPW in READ R1-5).

READ R1-5 (3E10.0)

LIST: PBASE, DELPW, TDIS

PBASE Atmospheric or reference pressure at the wellheads, psi. This is used to convert absolute pressure to gauge pressure.

DELPW Incremental value of pressure (psi) over which wellbore calculations are to be performed. The pressure and temperature calculations in the wellbores proceed in increments. The length increment corresponding to DELPW is calculated, and the temperature change over each increment is evaluated.

TDIS Thermal diffusivity of the rock surface surrounding the wellbores, ft^2/hr .

READ R1-6 (4I5)

The number of entries in the viscosity and temperature tables are entered here. You should enter as many viscosity data as are available. You are required to enter at least one viscosity point for the resident fluid (conc. = 0) and one for the injection fluid (conc. = 1). These reference viscosity points should preferably be at the middle of the expected temperature range, and, if possible, both reference viscosities should be entered at the same temperature. If only one viscosity point is available, the program obtains additional viscosity at other temperatures according to Lewis and Squires generalized chart. If you desire to enter a constant viscosity for any of the two fluids, you must enter one more viscosity point in addition to the reference viscosity. For example, if you desire to enter constant viscosity of 0.9 cp for the injection fluid, enter NTVI=1, the reference viscosity of the injection fluid VISIR=0.9 and VISI(1)=0.9.

The temperature table describes the initial temperature existing in the aquifer. For example, this table allows entry of existing geothermal gradients.

NOTE: Number of entries in the viscosity tables refers to the viscosity values to be entered in addition to the reference viscosities.

LIST: NCV, NTVR, NTVI, NDT

NCV Number of entries in the concentration-viscosity table. This table is for viscosities at the reference temperature TRR. The table should contain the viscosities of the fluid mixture at concentration other than 0 and 1, since these two values are entered as reference viscosities. If only the two pure fluid viscosities are available, enter zero and read in the viscosities of the pure fluids as reference viscosities.

NTVR Number of entries in the temperature-viscosity table for the aquifer resident fluid. This table is for viscosities other than at reference temperature TRR.

NTVI Number of entries in the temperature-viscosity table for the injection fluid. This table is for viscosities other than at the reference temperature TIR.

NDT Number of entries in the depth versus temperature table.

READ R1-7 (4E10.0)

LIST: TRR, VISRR, TIR, VISIR

The reference viscosities of the injection and the resident fluids are to be entered here.

TRR Reference temperature for the resident fluid viscosity, °F.

VISRR Viscosity of the resident fluid at the reference temperature TRR, cp.

TIR Reference temperature for the injection fluid viscosity, °F. If possible, this temperature should be taken to be equal to TRR.

VISIR Viscosity of the injection fluid at TIR, cp.

READ R1-8 (8F10.0)

NOTE: If NCV=0, omit R1-8.

LIST: SC(I), VCC(I), I=1, NCV

SC Concentration, fraction.

VCC Viscosity (cp) of a fluid mixture at concentration SC, and temperature TRR.

READ R1-9 (8F10.0)

NOTE: If NTVR=0, skip R1-9 and proceed to READ R1-10.

LIST: TR(I), VISR(I), I=1, NTVR

TR Temperature, °F.

VISR Viscosity (cp) of the resident fluid at the temperature TR. Do not re-enter the reference viscosity at TRR.

READ R1-10 (8F10.0)

NOTE: If NTVI=0, skip R1-10 and proceed to R1-11.

LIST: TI(I), VISI(I), I=1, NTVI

TI Temperature, °F.

VISI Viscosity (cp) of the injection fluid at the temperature TI. Do not re-enter the reference viscosity at TIR.

READ R1-11 (2F10.0)

Initial temperatures in the aquifer and the overburden-underburden blocks are to be entered here. The initial temperature is assumed to be a function of depth only. One set of data is always required even when NDT is zero. Data should be entered in the order of increasing depth.

Local horizontal and vertical variations in initial temperatures can be introduced in the aquifer in READ I-3. Initial temperature variations in the overburden and underburden blocks are not permitted in READ I-3. Regions unaltered by READ I-3 will retain initial temperature values calculated from data introduced in the depth-temperature table.

LIST: ZT(I), TD(I), I=1, NDT

ZT Depth, ft.

TD Temperature, °F.

READ R1-12 (2I5)

LIST: NZOB, NZUB

NZOB Number of overburden blocks. If NZOB is greater than 2 the heat loss calculations are performed.

NZUB Number of underburden blocks. If you desire the underburden heat loss calculations to be performed, a value of 3 or greater should be entered. If the number of aquifer blocks (NZ) is equal to one, the underburden heat loss is assumed to be equal to the overburden heat loss.

READ R1-13 (4E10.0)

LIST: KOB, CPOB, KUB, CPUB

KOB, KUB Vertical thermal conductivities of the overburden and the underburden blocks, respectively. These thermal conductivities should be entered in the same units as in READ R1-2.

CPOB, CPUB Overburden and underburden heat capacities per unit volume, Btu/(ft³-°F).

READ R1-14 (7E10.0)

These data are used to calculate the node spacing used in the overburden (underburden in READ R1-15) heat loss calculations. The calculated node spacing is printed in the program output.

NOTE: Skip this READ if NZOB=0

LIST: DZOB(K), K=1, NZOB

DZOB Thickness of each overburden block. The overburden block numbers increase as you go away from the aquifer.

READ R1-15 (7E10.0)

NOTE: Skip this read if NZUB=0.

LIST: DZUB(K), K=1, NZUB

DZUB Thickness of each underburden block. The block numbers increase as you go away from the aquifer.

READ R1-16 (4E10.0)

LIST: T0, PINIT, HINIT, HDATUM

T0 A standard temperature (°F) for calculating fluid density. Fluid density at any other temperature is calculated as the sum of the density at T0 and the deviation from it.

PINIT Initial pressure at reference depth HINIT, psi.

HINIT Reference depth for setting up initial conditions, ft. HINIT can be any depth within the reservoir.

HDATUM A datum depth (ft) for printing the dynamic pressures ($p - \rho gh/g_c$). The depth h is measured from the datum depth HDATUM.

The information read here is used in conjunction with DEPTH in READS R1-20 or R1-22 to establish the datum for printing pressure output. The DEPTH value (positive downward) locates the top of the grid block 1, 1, 1, with respect to a datum plane. HINIT is the reference depth measured from the datum plane at which the initial pressure is PINIT, and HDATUM is a depth relative to the datum at which the dynamic pressure is printed. For example, if DEPTH = 10.0 ft, the depth to the top of grid block 1, 1, 1, relative to a datum plane is 10 ft below the datum plane (Figure D-1). For a linear grid with NZ = 1, and $SINX = SINY = 0.0$ (READ R1-20), and PINIT = 4.9 psi, HINIT = 11.25 ft, HDATUM = 0.0, DZ(1) = 2.5 ft, with fluid density of 62.4 lbm/ft³, the INITIAL PRESSURE AT ELEVATION H is 4.3 psi. If the atmospheric pressure is specified as zero, and the fluid flow is static, PRESSURE AT ELEVATION H (PSIA) is 4.3 psi, and PRESSURE AT DATUM (PSIA) is 0.0 psi. If the absolute pressure is to be included, PINIT should be calculated as the static pressure of the overlying fluid plus the atmospheric pressure.

For NZ > 1, the static pressure of the nodes below the first node in the z-direction is calculated by adding a pressure increment based on the thickness and density of the next layer of fluid.

Temperature and solute concentration results are printed at elevation H. Density, viscosity, and enthalpy are printed at elevation H.

Figure D-1. Diagram of initial parameters.

READ R1-17 (7E10.0)

NOTE: If HTG = 3 (radial geometry), skip to READ R1-22.

LIST: DELX(I), I=1, NX

DELX Length of each row of blocks in the x-direction, ft.

READ R1-18 (7E10.0)

LIST: DELY(J), J=1, NY

DELY Length of each row of blocks in the y-direction, ft.

READ R1-19 (7E10.0)

LIST: DELZ(K), K=1, NZ

DELZ Thickness of each vertical layer, ft.

If you use the "homogenous" aquifer option (HTG = 1 in READ M-3) then the reservoir is treated as a rectangular parallelepiped. The grid defined by DELX, DELY, and DELZ values are the cell dimensions in the parallelepiped. The x-y plane of the grid is horizontal only if SINX and SINY of READ R1-20 are both zero. Similarly, the z-axis in this case points downward only if SINX and SINY are both zero. DELX and DELY are measured along the x-y plane and DELZ is perpendicular to the x-y plane.

If you use the "heterogenous" aquifer option (HTG = 2 in READ M-3), then the x-y plane is a horizontal plane placed over the aquifer structure. The x-axis should be aligned with the longer dimension of the aquifer and should be as "parallel" as possible with this longer dimension.

READ R1-20 (7E10.0)

NOTE: These data are read only if HTG = 1, and by themselves describe a homogenous reservoir. Heterogeneity may be introduced by using either READ R1-21 instead of R1-20 or by regional modifications in READ R1-27.

LIST: KX, KY, KZ, PHI, SINX, SINY, DEPTH

KX Hydraulic conductivity in the x-direction, ft/day. This quantity represents the fluid velocity obtained by a potential gradient of unity (ft. of water/ft.) of aquifer fluid of concentration zero and temperature T₀. In terms of permeability, this quantity is $(k\rho_0 g)/(g_c \mu_0)$. The parameters ρ_0 and μ_0 are the density and the viscosity of the aquifer fluid at concentration zero and temperature, T₀ (and P₀ = PINIT for density).

KY Hydraulic conductivity in the y-direction, ft/day.

KZ Hydraulic conductivity in the z-direction, ft/day.

- PHI Porosity in terms of a fraction. Porosity is the volume of voids over the total volume.
- SINX Sine of the reservoir dip angle along the x-axis.
- SINY Sine of the reservoir dip angle along the y-axis.
- DEPTH Depth from arbitrary reference plane (e.g. sea level) to the top of grid block (1,1,1), feet, measured positive downward.

READ R1-21 (3I3,1X,7E10.0) or (LIST 1-6I5,LIST 2-6E10.0)

NOTE: These data are read only if HTG = 2. Two input formats are permissible. The first allows for aquifer modification on a single block, and the second allows modification over a series of grid blocks. The first format is accessed by default. If the second format is desired, enter -1 in place of I in the first format and proceed to enter data in the form of the second format.

LIST: I, J, K, KX, KY, KZ, PHI, UH, UTH, UCPR

I,J,K Grid block indices. If I is -1, proceed to the second format.

KX x-direction hydraulic conductivity for flow, ft/day.

KY y-direction hydraulic conductivity for flow, ft/day.

KZ z-direction hydraulic conductivity for flow, ft/day.

PHI Porosity, in terms of a fraction.

UH Depth (feet) measured positively downward from the reference plane to top of the cell. This has the same definition as READS R1-20 and R1-22.

UTH Grid block thickness in the vertical direction, ft. If the layer thickness is equal to DELZ(K) read in under R1-19, UTH may be entered as zero.

UCPR Heat capacity of rock per unit volume, Btu/(ft³-°F). If the rock heat capacity is equal to CPR (READ R1-1), UCPR may be entered as zero.

You must read one card for each non-zero pore volume block. Cards need not be included for zero pore volume blocks within the grid. If you desire a change in the input format from a single data entry after a series of single block data entries, enter - 1 in the I position and enter data using the second format on the next series of cards. Follow the last card with a blank card and proceed to READ R1-26.

NOTE: This section offers a means of entering data on a large number of blocks. This section is activated by first entering I as -1 in READ R1-21, followed by the data in the second input format. Data for

regions of zero pore volume blocks need not be included. Enter as many of these data as necessary, and follow the last set by a blank card.

LIST: I1, I2, J1, J2, K1, K2,

KX, KY, KZ, PHI, UH, UTH, UCPR

I1, I2 Lower and upper limits inclusive, on the I-coordinate of the region.

J1, J2 Lower and upper limits inclusive, on the J-coordinate of the region.

K1, K2 Lower and upper limits inclusive, on the K-coordinate of the region.

KX, KY, KZ Hydraulic conductivities in x, y, and z-directions, respectively, ft/day.

PHI Porosity, fractional.

UH Depth to top of region. If entered as zero, it is not modified. This has a similar definition as DEPTH in READS R1-20 and R1-22.

UTH Grid block thickness in the vertical direction, ft. If the layer thickness is equal to DELZ(K) read in under R1-19, UTH may be entered as zero.

UCPR Heat capacity of rock per unit volume, Btu/(ft³-°F). If the rock heat capacity is equal to CPR (READ R1-1), UCPR may be entered as zero.

READ R1-22 (4E10.0)

NOTE: Skip to READ R1-26 if HTG is not equal to 3.

These data are read for radial geometry aquifer with only one injection or production well. The well is located at the center of the numerical block system. The grid blocks are divided on the equal $\Delta \log(r)$ basis, i.e., r_i/r_{i-1} is constant or, by entering individual grid block center radii in READ R1-26. If you desire to use regions of equal $\Delta \log(r)$ instead of a constant value of $\Delta \log(r)$ throughout the aquifer, you should specify the number of blocks in each region (READ R1-24) and the external boundaries between the regions (READ R1-25). If you desire to enter grid block centers, set R1=0.

LIST: RWW, R1, RE, DEPTH

RWW Well radius, ft.

R1 Grid block entry selection and distance from the edge of the grid system to first grid block center, ft.

>0 - Distance to first grid block, ft. Grid block sizes will be allocated on an equal $\log(r_i/r_{i-1})$ basis.

0 - Grid block center values will be read in READ R1-26.

RE External radius of the aquifer, ft.

DEPTH Depth from a reference plane to the top of the aquifer, ft.

READ R1-23 (5E10.0)

LIST: DELZ(K), KYY(K), KZZ(K), POROS(K), CPR1(K), K=1, NZ

DELZ Layer thickness in the vertical direction, ft.

KYY Horizontal hydraulic conductivity, ft/day.

KZZ Vertical hydraulic conductivity, ft/day.

POROS Porosity, in terms of a fraction.

CPR1 Rock heat capacity, Btu/(ft³-°F). If the rock heat capacity in the layer is equal to CPR (READ R1-1), CPR1 may be entered as zero.

You must enter one card for each vertical layer.

Note: If R1 = 0, skip READS R1-24 and R1-25, and proceed directly to READ R1-26.

READ R1-24 (5I5)

NOTE: These data are read for obtaining regions of equal $\Delta \log(r)$. If you desire a constant value of $\Delta \log(r)$ throughout the aquifer, insert a blank card and proceed to READ R1-27.

LIST: NXR(I), I=1, 5

NXR Number of grid blocks in each $\Delta \log(r)$ region. You may specify as many as five regions. The total number of grid blocks in all the regions cannot exceed NX. The number of blocks in the outer most region need not be specified. For example, if you desire a total of 25 radial grid blocks and three regions of 5, 10 and 10 grid blocks, then enter NX = 25 (READ M-3) and NXR's may be entered as 5, 10, 0, 0, 0 or as 5, 10, 10, 0, 0.

READ R1-25 (5E10.0)

NOTE: If NXR(1) > 0, this card is required.

LIST: RER(I), I=1, 5

RER Radii of the external boundaries between different regions, ft. As an example, if the external radius of the aquifer is 5,000 feet and you require five grid blocks in the first 1,000 feet, 10 grid blocks from 1,000 to 2,500 feet, and 10 grid blocks from 2,500 to 5,000 feet and if you entered NXR's as 5 and 10 (and the rest as zeros), you should enter RER's as 1,000 and 2,500 feet only (the rest as zeros). Alternatively, if NXR's were specified as 5, 10 and 10, then RER's should be entered as 1,000, 2,500 and 5,000.

NOTE: If $R1 > 0$, proceed to READ R1-27.

READ R1-26 (7E10.0)

LIST: RR(I), I=1,NX

RR Grid block center radius, feet.

READ R1-27 (LIST 1 - 6I5, LIST 2 - 6E10.0)

NOTE: Read as many of these data as necessary to describe all the reservoir description modifications desired. Follow the last set with a blank card, which the program recognizes as the end of this data set. Even if no regional modifications are desired, the blank card must nevertheless be included.

LIST 1: I1, I2, J1, J2, K1, K2

LIST 2: FTX, FTY, FTZ, FPV, HADD, THADD

I1,I2 Lower and upper limits inclusive, on the I-coordinate of the region to be modified.

J1,J2 Lower and upper limits inclusive, on the J-coordinate of the region to be modified.

K1,K2 Lower and upper limits inclusive, on the K-coordinate of the region to be modified.

FTX If positive or zero, this is the factor by which the x-direction transmissibilities within the defined region are to be multiplied. If negative, the absolute value of FTX will be used for the x-direction transmissibilities within the region to be modified, replacing the values read in earlier or determined from the permeability data read in earlier.

FTY This has the same function of FTX, but applies to the y-direction transmissibilities.

FTZ This has the same function of FTX, but applies to the vertical direction transmissibilities.

FPV This has the same function as FTX, but applies to the pore volumes.

HADD This is an increment that will be added to the depths within the defined region. A positive value repositions the cell deeper, and a negative value brings it closer to the surface.

THADD This is an increment added to the thickness values within the defined region. A positive value makes the cell thicker and a negative value makes it thinner.

This data modification procedure provides the user with an easy way to build in reservoir heterogeneities or modify the reservoir description data during history matching. These modifications are applicable regardless whether the data were read according to READ R1-20, R1-21, or R1-23.

The modifiers in LIST 2 above are independent in a way that a change effected by any one of them does not affect any other properties. For example, an FPV of 1.4 will increase the pore volume by 40%, but will not result in any changes in transmissivities, depth, or thickness.

The data modifications will occur over rectangular regions areally as defined by I1, I2, J1, and J2 limits. The vertical extent of the region is defined by K1 and K2. All six of these limits must be within the calculation grid. Successive regions may be partially or entirely overlap other regions.

In regions in which one or more modifications have been made to a parameter is subjected to additive modifications, and the order of modifications has no effect and the final net adjustment is simply the algebraic sum of all the additive factors that apply to the region. For the transmissibility and pore volume modifications, the order multiple changes does not affect the final result if all the modifiers are multiplicative (positive). However, if some or all of the modifications are replacement values, (negative entry) the order of the input may effect the final result. For example, consider the following two situations in which the same modification data are applied in different orders to an original value and the final result is different.

TYPE	CASE 1	CASE 2
Original value	100	100
Modification and Result	.50(50)	-70.(70.)
Modification and Result	-70.(70.)	.50(35.)
Modification and Result	.20(14.)	.20(7.)

The program will accept a zero modifier as a valid parameter. Therefore, if no changes are desired to data that are affected by multiplicative factors (FTX, FTY, FTZ and FPV) read the corresponding as 1.0, not zero. Zero additive factors (HADD and THADD) result in no changes to the depth and thickness values.

A modification to the transmissibilities over the region (I1-I2, J1-J2, and K1-K2) will not affect the transmissibilities between columns I2 and I2+1, between the rows J2 and J2+1 or between layers K2 and K2+1.

READ R1-28 (2I5)

NOTE: If the aquifer influence functions are zero, insert a blank card and proceed to READ I-1.

LIST: IAQ, PRTAB

IAQ Control parameter for selecting the type of aquifer block representation.

0 - No aquifer influence blocks are to be used. Skip to READ I-1.

- 1 - A pot aquifer representation will be used.
- 2 - A steady-state aquifer representation will be used.
- 3 - Use the Carter-Tracy representation.

PRTAB Print control key for the aquifer influx coefficient.

- 0 - No printing of aquifer influx coefficients will be activated.
- 1 - The locations and values of the aquifer influx coefficients will be printed.

NOTE: Aquifer influence blocks are defined as those cells in the model that communicate directly with an aquifer that is not modeled as part of the calculation grid, but whose effects are introduced through the aquifer terms read here. This feature can be used to introduce water influx (or efflux) from an edge or bottom water drive without the expense that would be required to model the aquifer as part of the grid system. For example, an infinite aquifer can be modeled without using an infinitely large grid network. The chosen aquifer influence function is attached to the periphery of the grid network, outside the the region of interest.

If HTG =3, aquifer influence blocks are assigned to the last areal plane K=1,2,3, ... NZ, by default.

READ R1-29 (LIST 1 - 6I5, LIST 2 - E10.0)

NOTE: These data are read only if IAQ is 1 or 2, meaning the pot or steady-state aquifer has been selected. If IAQ is 3, omit this READ and proceed to READ R1-30.

LIST 1: I1, I2, J1, J2, K1, K2

LIST 2: VAB

I1,I2 Lower and upper limits, inclusive, on the I-coordinate of the aquifer influx region.

J1,J2 Lower and upper limits, inclusive, on the J-coordinate of the aquifer influx region.

K1,K2 Lower and upper limits, inclusive, on the K-coordinate of the aquifer influx region.

VAB Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The units of VAB are ft³/psi for a pot aquifer representation, and ft³/psi-day for a steady-state representation.

NOTE: Follow the last VAB card of this data group by a blank card.

The READ group consists of two cards, each set defining a rectangular region and the value of VAB to be assigned to that region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set read to be assigned to the overlapped subregion. If these data are read, i.e. IAQ=1 or 2, then skip READ R1-30 through R1-33 and proceed to READ R1-34.

READ R1-30 (3I5)

NOTE: If IAQ is not equal to 3, omit these data and proceed to READ R1-34. This section is used to enter data for the Carter-Tracy method of calculating aquifer influence functions.

If HTG = 3, the program assigns VAB=1.0 to each edge perimeter block by default. If you desire to change this, enter NCALC = 0, and read in new locations and VAB in READ R1-31, and modify the default VAB to zero using READ R1-34. If HTG = 3, and NCALC = 2, the program will ignore NCALC = 2, and assign VAB to each perimeter block.

LIST: NCALC, NPT, PRTIF

NCALC Control parameter for selecting how the Carter-Tracy aquifer coefficients are to be assigned.

- 0 - The Carter-Tracy aquifer coefficients (VAB) will be read in as input data.
- 1 - The VAB will be calculated by the program and assigned to each edge (perimeter) block in each areal plane, $K = 1, 2, \dots, NZ$.
- 2 - The VAB will be calculated by the program and assigned to each grid block in the lower-most areal plane $K = NZ$ only.

NPT Number of points in the influence function vs. dimensionless time table, $(P_d(t_d) \text{ vs. } t_d)$. If NPT is zero, the program will select the Hurst-Van Everdingen infinite aquifer solution internally.

PRTIF Print control key for the influence function table.

- 0 - Suppress printing.
- 1 - Print the table of $P_d(t_d) \text{ vs. } t_d$.

READ R1-31 (LIST 1 - 6I5, LIST 2 - E10.0)

NOTE: Enter these data if NCALC is zero; otherwise, skip this READ and proceed to READ R1-32.

LIST 1: I1, I2, J1, J2, K1, K2

LIST 2: VAB

- I1,I2 Lower and upper limits, inclusive, on the I-coordinate of the aquifer influence region.
- J1,J2 Lower and upper limits, inclusive, on the J-coordinate of the aquifer influence region.
- K1,K2 Lower and upper limits, inclusive, on the K-coordinate of the aquifer influence region.
- VAB Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The aquifer influence coefficient VAB for the Carter-Tracy method is actually the fraction of the total aquifer-reservoir boundary that is represented by the length of any given grid block. For this reason, it is possible to calculate the VAB from the input data previously read in, and the VAB does not have to be calculated externally.

NOTE: Follow the last VAB card of this data group by a blank card.

The read group consists of two cards or any number of sets of two cards, each set defining a rectangular region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set read to be assigned to the overlapping subregion.

READ R1-32 (4E10.0)

LIST: KH, PHIH, RAQ, THETA

- KH Conductivity-thickness for aquifer, ft^2/day . An average value of transmissivity should be used.
- PHIH Porosity-thickness for the aquifer, ft.
- RAQ Equivalent aquifer radius, ft. The approximate method of Carter and Tracy is valid for circular aquifers. To retain the validity of usage of circular reservoir influence functions, the numerical grid system should be chosen as square as possible.
- THETA Angle of influence, degrees. This angle should indicate the portion of the aquifer covered by the aquifer influence boundary. If mass flow is permitted across all external boundaries, enter 360° .

READ R1-33 (2F10.0)

NOTE: This data is entered if NPT is not equal to zero. If NPT is zero, the program will select the aquifer influence functions for an infinite aquifer, and you do not have to read in the influence function data. Omit this READ and proceed to READ R1-34.

LIST: TD(I), PTD(I), I=1, NPT

- TD Dimensionless time, $kt/(\mu\phi c_t r_e^2)$.

PTD Terminal rate case influence function as given by Van Everdingen and Hurst.

READ R1-34 (LIST 1 - 6I5, LIST 2 - E10.0)

LIST 1: I1, I2, J1, J2, K1, K2

LIST 2: FAB

NOTE: These data allow the user to modify the aquifer influx coefficient VAB by the relation

$$VAB(I,J,K) = VAB(I,J,K) \times FAB.$$

This is useful when a reservoir may experience no or limited water influx across one boundary. In this case, in the region where the influx is limited, the FAB may be set to zero or a small number to reduce the VAB along the boundary.

I1,I2 Lower and upper limits, inclusive, on the I-coordinate of the VAB to be modified.

J1,J2 Lower and upper limits, inclusive, on the J-coordinate of the VAB to be modified.

K1,K2 Lower and upper limits, inclusive, on the K-coordinate of the VAB to be modified.

FAB Factor by which the VAB will be modified in the region $I = I1, I2, J = J1, J2$, and $K = K1, K2$.

NOTE: Follow these data with one blank card. If no modifications are desired, one blank card is still required.

READ I-1 (3I5)

NOTE: These data are read for initializing concentrations, natural flow, and temperature in the aquifer. If the initial concentrations are zero everywhere in the aquifer, if there is no natural flow, and if temperature is to be initialized by the temperature table in READ R1-11, insert a blank card and proceed to READ R2-1.

LIST: ICOMP, INAT, ITEMP

ICOMP Control parameter for initializing the concentrations.

0 - Initial concentrations in all the grid blocks are zero. If you enter zero, skip READ I-2.

1 - The initial concentrations are not zero everywhere. Non-zero concentrations will be entered in READ I-2.

INAT Control parameter for entering natural fluid velocity.

0 - The aquifer fluid is static initially. If you enter zero skip READ I-4.

1 - The resident fluid velocity will be entered in READ I-4.

ITEMP Control parameter for initial temperatures in the aquifer assigned by regional basis.

0 - Initial temperatures in all grid blocks are assigned by a vertical temperature profile entered in READ R1-11.

1 - Temperature variations in the temperature profile will be introduced by the user in READ I-3.

READ I-2 (6I5, F10.0)

NOTE: Skip this READ if ICOMP is zero.

LIST: I1, I2, J1, J2, K1, K2, CINIT

I1,I2 Lower and upper limits, inclusive, on the I-coordinate of the non-zero concentration region.

J1,J2 Lower and upper limits, inclusive, on the J-coordinate of the non-zero concentration region.

K1,K2 Lower and upper limits, inclusive, on the K-coordinate of the non-zero concentration region.

CINIT Initial concentration in each of the of the blocks within the region defined by I1, I2, and etc., dimensionless.

NOTE: Read as many of these cards as necessary to describe the concentrations everywhere in the aquifer. You need to specify only the non-zero concentrations. Follow the last card with a blank card.

READ I-3 (6I5, F10.0)

NOTE: Skip this READ if ITEMP is zero.

LIST: I1, I2, J1, J2, K1, K2, TINIT

I1,I2 Lower and upper limits, inclusive, on the I-coordinate of the region of temperature initialization.

J1,J2 Lower and upper limits, inclusive, on the J-coordinate of the region of temperature initialization.

K1,K2 Lower and upper limits, inclusive, on the K-coordinate of the region of temperature initialization.

TINIT Initial temperature in each of the of the blocks within the region defined by I1, I2, and etc., °F.

NOTE: Read as many of these cards as necessary to describe the temperatures everywhere in the aquifer. Regions not modified will retain initial temperature assigned in READ R1-11. Follow the last card with a blank card.

READ I-4 (F10.0)

NOTE: If INAT = 0, skip this card.

LIST: VEL

VEL Initial velocity of the resident aquifer fluid in the x-direction, ft/day (Darcy velocity). The initial velocities in the y- and z-directions are assumed to be zero.

RECURRENT DATA

The data described previously are required to describe the aquifer and fluid properties and to establish initial conditions. The recurrent data are read before the first time step and at subsequent time steps when you desire to change the well conditions, time step data, or mapping specifications. Note that any of the data entered up to this point cannot be changed. The overburden and underburden blocks specifications or aquifer influence functions cannot be changed in any manner once they have been specified at the beginning.

READ R2-1 (7I5)

LIST: INDQ, IWELL, IMETH, ITHRU, IPROD, IOPT, INDT

INDQ Control parameter for reading well rates.

- 0 - Do not read well rates.
- 1 - Read well rates on one card (READ R2-5). The user must enter all well rates under this option.
- 2 - Read one card for each well rate (READ R2-6).

IWELL Control parameter for reading well definition data.

- 0 - Do not read well data.
- 1 - Read new or altered well data.

IMETH Control parameter for reading method of solution.

- 0 - Do not read method of solution. If you are entering data the first time run (new run) and you enter IMETH=0, the program selects direct solution backward with time and space finite difference approximations. The solution under these conditions is unconditionally stable.

- 1 - Read new or altered method of solution.

ITHRU Run termination control.

- 0 - Run is to continue.
- 1 - Run is to terminate at this point. No more recurrent data will be read after this card. If you do not desire any plots, i.e. NPLP, NPLT and NPLC are all zero, this should be your last card in your data deck.

IPROD Control parameter for reading wellbore data.

- 0 - Do not read wellhead data.
- 1 - Read new or altered wellhead data.

IOPT Control parameter for reading wellbore iteration data.

- 0 - Do not read wellbore iteration data. If it is a new run and you desire the wellbore calculations to be performed, default values of iteration parameters will be used for wellbore calculations.
- 1 - Read new or altered wellbore iteration data.

INDT Control parameter for reading reservoir solution iteration data.

- 0 - Do not read iteration data. If you are entering data before the first time step, default values of iteration parameters will be used.
- 1 - Read new or altered iteration data.

READ R2-2 (I5,F10.0)

NOTE: This data is entered if IMETH is not equal to zero. If it is a new run and IMETH is equal to zero, the program selects METHOD=1 and WTFAC=1.0 (direct solution with backward space and time approximations).

LIST: METHOD, WTFAC

METHOD Method of solution. If you enter zero, the program selects METHOD=1. You may select direct solution only if you specified direct solution in READ M-3.

- 1 - Reduced band width direct solution with backwards finite-difference approximation in time.
- 2 - Two-line successive overrelaxation (L2SOR) solution with backward finite-difference approximation in time.

- 1 - Reduced width direct solution with Crank-Nicholson approximation in time.
- 2 - Two-line successive overrelaxation solution with Crank-Nicholson approximation in time.

WTFAC Weight factor for finite-difference approximation in space.

1.0 - Backward difference.

0.5 - Central difference.

If you enter $WTFAC \leq 0$, the program selects $WTFAC = 1.0$.

READ R2-3 (I5, 4F10.0)

NOTE: This data is entered if IOPT is greater than zero. If you intend to use the default values, insert a blank card and proceed to READ R2-4. The default values of the parameters are discussed below.

LIST: NITQ, TOLX, TOLDP, DAMPX, EPS

- NITQ Maximum number of outer iterations in the wellbore calculations. For example, if the injection rate for a well is specified, the wellhead pressure is calculated iteratively to obtain the bottom-hole pressure necessary to inject the specified rate. If entered as zero or negative number, the program selects the default value of 20.
- TOLX The tolerance on the fractional change in pressure over an iteration. If entered as zero or a negative number, the default value of 0.001 is selected.
- TOLDP The tolerance on pressure, psi. The default value is 1.0 psi.
- DAMPX Damping factor in estimating the next value of the pressure (surface for an injection well and bottom-hole for a production well). If the frictional pressure drop in the well is high, a linear extrapolation may lead to oscillations around the right value. The default value is 2.0.
- EPS The tolerance on calculating temperature from given values of enthalpy and pressure. The fluid temperatures in the wellbore are calculated over each pressure increment as specified in READ R1-3. The default value is 0.001.

READ R2-4 (I5)

NOTE: If INDQ is equal to zero, skip READ R2-4 through R2-6 and proceed to R2-7. This data is required if INDQ is not zero.

LIST: NWT

NWT Total number of wells.

READ R2-5 (7E10.0)

NOTE: Enter this data only if INDQ is equal to one.

LIST: Q(I), I=1, NWT

Q Production rate, ft^3/day . If it is an injection well, enter the value as a negative production rate. You must enter all the well rates even if all of them have not changed.

READ R2-6 (I5, E10.0)

NOTE: Enter this data only if INDQ is equal to two. Read as many cards as necessary to describe all the injection and production well rates. Follow the last card with a blank card.

LIST: I, QWELL

I Well number.

QWELL Production rate, ft^3/day . Enter negative values for injection rates. You need to enter only the altered well rates.

READ R2-7 (LIST 1 - 6I5, LIST 2 - 4E10.0, LIST 3 - 8E10.0 and LIST 4 - 7E10.0)

NOTE: This data is entered for IWELL equal to one. Read one set of data for each well and follow the last card with a blank card.

LIST 1: I, IIW, IJW, IIC1, IIC2, IINDW1

I Well number.

IIW I-coordinate of grid cell containing the well.

IJW J-coordinate of grid cell containing the well.

IIC1 Uppermost layer in which the well is completed.

IIC2 Lowermost layer in which the well is completed.

IINDW1 Well specification option.

- 1 - Specified rate is allocated between layers on the basis of mobilities alone.
- ±2 - Specified rate is allocated between the layers on the basis of mobilities and the pressure drop between the wellbore and the grid block.
- ±3 - An injection or production rate is calculated from the specified bottom-hole or surface pressure. The lower of the specified and the calculated rate is allocated between layer on the basis of mobilities and the pressure drop between the wellbore and the grid block.

2,3 - The rate is expressed explicitly in the aquifer model equations.

-2,-3 - The rate is expressed in a semi-implicit manner in the aquifer model equations, e.g.,

$$q^{n+1} = q^n + dq/dp (p^{n+1} - p^n)$$

LIST 2: WI, BHP, TINJ, CINJ

WI Well index, ft²/day.

BHP Bottom-hole pressure, psi. This must be specified if IINDW1 = ±3.

TINJ Temperature of the injection fluid, °F. If surface conditions are being specified, it is the temperature at the surface.

CINJ Contaminant concentration in the injection fluid, dimensionless.

LIST 3: X, DW, ED, OD, TTOPW, TBOTW, UCOEF, THETA

NOTE: Skip this list if ISURF = 0.

X Pipe (wellbore) length to top of perforations, ft.

DW Inside wellbore (pipe) diameter, ft.

ED Pipe roughness (inside), ft. Enter zero if it is a smooth pipe.

OD Outside wellbore (casing) diameter, ft.

TTOPW Rock temperature surrounding the wellbore at the surface, °F.

TBOTW Rock temperature surrounding the wellbore at the bottom-hole, °F.

UCOEF Overall heat transfer coefficient between the inner surface of the pipe and outer surface of the casing, Btu/ft²-°F-hr.

THETA Angle of the wellbore with the vertical plane, degrees.

LIST 4: KHL(K), K = IC1, IC2

NOTE: Skip this READ if the well completed in only one layer, i.e. IIC1 = IIC2.

KHL(K) Layer allocation factors for Well I. These should be in proportional to total productivity of individual layers, taking into account layer kh (absolute transmissivity x thickness) and layer formation damage or improvement (skin). Only the relative values of these factors are important. For example, if layers 3 through 6 (IC1=3, IC2=6) are completed, then KHL values of .5, 2, 2.5, .1 will

give the same result as values of 5, 20, 25, 1. The absolute productivity (injectivity) of completion layer K is computed as

$$WI \times KHL(K+1-IC1) / \sum_{l=1}^{l=IC2-IC1+1} KHL_l$$

READ R2-8 (7E10.0)

NOTE: Skip this read if IPROD is zero.

LIST: THP(I) I =1, NWT

THP Tubing hole or surface pressure for each well, psi. If ISURF is one, THP must be specified for the wells with well option IINDW1=±3. A production or injection rate is calculated from THP, and lower of the calculated and specified rate is used for allocation between layers.

READ R2-9 (3I5)

This data is entered if INDT is not zero. If you desire to use the default values for the data entered on this card, enter INDT as zero and skip this READ. However, if you desire to include the off-diagonal (or cross derivative) dispersion terms in the x-y plane (E_{xy} and E_{yx}), MINITN must be entered greater than or equal to 2. If MINITN is entered as one, or if the default value is used, an approximation is used to include the effect of the off-diagonal terms by enhancing the diagonal terms.

LIST: MINITN, MAXITN, IMPG

MINITN Minimum number of outer iterations in the subroutine ITER. The default value has been programmed as one.

MAXITN Maximum number of outer iterations in the subroutine ITER. The default value is 5.

IMPG Number of time steps after which the optimum parameters for the inner iterations are recalculated for the two line successive over-relaxation method. You do not have to enter this data if METHOD is not equal to ±2. The default value for IMPG is 5.

READ R2-10 (7E10.0)

LIST: TCHG, DT, DSMX, DPMX, DTPMX, DTMAX, DTMIN

TCHG Time (days) at which next set of recurrent data will be read. The restart record can be written at TCHG only. Also, the mapping subroutine can be activated at TCHG only.

DT Time step specification. If DT is positive it will be the time step (days) used from the current time to TCHG. If DT is zero, the program will select the time step automatically. DT must not be zero for the first time step of a run starting from zero time.

- DSMX Maximum (over entire grid) concentration change desired per time step.
- DPMX Maximum (over entire grid) pressure change desired per time step, psi.
- DTPMX Maximum (over entire grid) temperature change desired per time step, °F.
- DTMAX Maximum time step allowed (days).
- DTMIN Minimum time step required (days).

If any of the five parameters above is entered as zero, default values are used. These values are listed as follows:

DSMX = 0.25

DPMX = 50.0 psi

DTPMX = 10.0 °F

DTMAX = 30.0 days

DTMIN = 1.0 day

These parameters are used only if DT equals zero. The time step DT must not be read as zero for the first time step. If DT is read as zero, the program will automatically increase or decrease the time step size every time step to seek a value such that the maximum changes in the concentration, pressure, and temperature are less than or equal to the specified values.

READ R2-11 (10I5)

LIST: IO1, IO2, IO3, IO4, IO8, RSTWR, MAP, KOUT, MDAT, IIPRT

The program prints four types of output at the end of each time step. The parameters IO1, IO2, IO3, and IO4 control the frequency of the outputs.

- IO1 Control parameter for frequency of the time step summary output. The time step summary (7 lines) gives cumulative field injections and productions, material and heat balances, average aquifer pressure, cumulative heat loss to the overburden and the underburden, cumulative water, contaminant and heat influxes across the peripheral boundaries, and the maximum pressure, concentration, and temperature changes in any block during the time step.
- IO2 Control parameter for frequency of the well summary output. This summary gives water, heat and contaminant fluid production and injection rates, cumulative production and injection, wellhead and bottom-hole pressures, wellhead and bottom-hole temperatures and the grid block pressure in which the well is located. This summary also gives the total production and injection rates and cumulative production and injection.

- I03 Control parameter for listing of the grid block values of concentration, temperature, and pressure.
- I04 Control parameter for injection/production rate in each layer for each well.

The following apply to all four of the above parameters:

- 1 Omit printing for all time steps from the current time through to TCHG, inclusive.
 - 0 Print at the end of each time step through to the step ending at TCHG.
 - 1 Print only at time TCHG.
- n(>1) Print at the end of every n^{th} time step and at the time TCHG.
- I08 Control parameter for listing of the grid block values of the dependent variables. The listing is printed according to the frequency specified (I03). This parameter gives you the option for not printing the tables you do not desire. The parameter requires a three digit specification, and the first always refers to pressure, the second to temperature, and the third to concentration.
- 0 - The grid block values will be printed.
 - 1 - The grid block values (pressure at datum or temperature or concentration) will not be printed.
 - 2 - Refers to the first digit only. Neither the absolute pressure nor the pressure at datum will be printed.
 - 2 - Refers to the second digit only. Print overburden and underburden and reservoir grid block temperature values.
- e.g. If you desire only temperature grid block values, enter 201.

RSTR Restart control parameter.

- 0 - No restart record will be written.
- 1 - Restart record will be written on tape 8 at time TCHG.

MAP Parameter for printing contour maps at time TCHG. Only two-dimensional section maps are printed. The maps are printed for r-z coordinates in a radial system, x-z coordinates in a 2-dimensional profile problem, and x-y coordinates (areal maps) in a linear system. Three-dimensional maps are printed as a series of NZ two-dimensional section (areal) maps for each layer at elevation H. This parameter requires a three digit specification, the first digit referring to mapping pressures, the second for mapping temperatures, and the third for concentrations.

- 0 - The variable will not be mapped.
- 1 - The variable will be mapped at TCHG.
- e.g. If you desire the contour maps for pressure and temperature only, enter 110.

KOUT Output control (same as M-3).

- 0 - All program output activated.
- 1 - All program output except initial arrays (concentrations, pressures, etc.) are activated.
- 3 - No program output is activated.

MDAT Control parameter for entering the mapping specifications.

- 0 - The mapping specifications are not to be changed.
- 1 - Read new mapping specifications. If you are activating the printing of contour maps for the first time during the current run, MDAT must be entered as one.

IIPRT Transmissibilities, fluid properties, and Darcy velocities are activated by this print key (see READ M-2). Print tables activated by this print key are only printed at TCHG (READ R2-11).

- 0 - Print key output remains unchanged from its last entry through READ M-2 or R2-11.
- 1 - All transmissibilities, Darcy velocities and fluid properties at the old time level are printed.
- 2 - Only Darcy velocities calculated at the old time level are printed.
- 3 - Stop all output activated by IIPRT.

READ R2-12 (I5, 2F10.0)

NOTE: Enter this data if you desire contour maps (MAP is not equal to 000) and if MDAT is equal to one.

LIST: NORIEN, XLGTH, YLGTH

NORIEN Map orientation factor.

- 0 - The map is oriented with x (refers to r for radial geometry) increasing from left to right and y (z for radial geometry) increasing up the computer page, i.e. the x=0, y=0 point is at the lower left hand corner.

- 1 - The map is oriented with x increasing from left to right and y increasing down the computer page. The origin is the upper left hand corner. Maps in x-z (linear grid) profile view should be printed using this orientation factor.

XLGTH The length, in inches, on the computer output which is desired in the x (or r) direction.

YLGTH The length, in inches, on the computer output which is desired in the y (or z for radial geometry) direction.

READ R2-13 (6I5, 2F10.0)

NOTE: Enter this data only if pressure contour maps are desired and if MDAT equals one. These entries refers to pressure mapping only.

LIST: IP1, IP2, JP1, JP2, KP1, KP2, AMAXP, AMINP

IP1,IP2 Lower and upper limits, inclusive, on the I-coordinate of the region to be mapped. If IP1 and IP2 are both zero, the region to be mapped will extend from the first to the last node in the x-direction.

JP1,JP2 Lower and upper limits, inclusive, on the J-coordinate of the region to be mapped. If JP1 and JP2 are both zero, the region to be mapped will extend from the first to the last node in the y-direction.

KP1,KP2 Lower and upper limits, inclusive, on the K-coordinate of the region to be mapped. For a linear system, you will get (KP2 - KP1 +1) areal maps.

AMINP,AMAXP The minimum and maximum value of the pressure (psi) used to obtain 20 contour intervals. If the pressure in any grid block is higher than AMAXP, it will be indicated as AMAXP, and similarly a pressure lower than AMINP is printed as AMINP. If you enter AMAXP as zero or a negative value, the program will search for a maxima and use the value as AMAXP. If you enter AMINP as a large negative number (≤ -99.0), the program will search for the minima and use the value as AMINP.

READ R2-14 (6I5, 2F10.0)

NOTE: This READ refers to temperature contour maps. Enter this data only if temperature maps are desired, and if MDAT equals one.

LIST: IT1, IT2, JT1, JT2, KT1, KT2, AMAXT, AMINT

The user is referred to READ R2-13 for definition of these parameters. This card refers to temperature mapping only as opposed to pressure mapping for R2-13.

READ R2-15 (6I5, 2F10.0)

NOTE: This READ refers to concentration contour maps. Enter this data only if concentration maps are desired and if MDAT equals one.

LIST: IK1, IK2, JK1, JK2, KK1, KK2, AMAXK, AMINK

See READ R2-13 for definition of these parameters. This card refers to concentration mapping only as opposed to pressure mapping for READ R2-13.

NOTE: The data entered up to this point are sufficient to execute the program until time equal TCHG. The recurrent data are read again at that point. If you desire to terminate a run, enter ITHRU=1 (READ R2-1) after R2-15. If you desire any plots (if NPLP or NPLT or NPLC equals one), you should enter the plotting data (READ P-2 through P-4). If you do not desire any plots, ITHRU=1 will terminate execution at this point.

PLOTTING DATA

The specifications for the plots and observed data are entered here. You may obtain plots even if you do not have any observed data available. Do not enter any plotting data if you do not desire any plots. Plots can be obtained for the values of the dependent variables in the well (at the wellhead and at the bottom-hole). The quantities plotted depend upon the "type" of the well. The quantities plotted for different wells are as follows:

<u>Type of Well</u>	<u>Quantities Plotted</u>
Observation well	Bottom-hole pressure, temperature, and concentration
Injection well, bottom-hole conditions specified (ISURF=0)	Bottom-hole pressure
Injection well, surface conditions specified (ISURF=1)	Bottom-hole pressure and temperature, surface pressure
Production well, bottom-hole conditions specified	Bottom-hole pressure, temperature, and concentration
Production well, surface conditions specified	Bottom-hole pressure, temperature, and concentration, surface pressure and temperature.

You should enter READ P-1 only if you are obtaining plots for a previous run. The plotting data for one well consists of the data from READ P-2 through P-4. Enter as many of these sets of these data as the wells for which you desire plots. If you desire plots for all the wells, enter NWT sets of these data. If you enter less than NWT sets, follow these cards with a blank card.

READ P-1 (I5)

NOTE: Enter this data only if NPLP or NPLT or NPLC equals -1, i.e., the plots are desired for a previous run.

LIST: NWT

NWT Total number of wells.

READ P-2 (I5, 5X, 10A4)

LIST: KW, ID

KW The well number.

ID A title for the plots for well number KW.

READ P-3 (7E10.0)

LIST: TMN, TMX, DT, PWMN, PWMX, PSMN, PSMX, TWMN, TWMX, TSMN, TSMX, CMN, CMX

These variables define the ranges of the coordinate axes for plots.

TMN Lower limit on time.

TMX Upper limit on time.

DT Time step for each row. For example, if TMN=5, TMX=15, and DT=0.5, the time coordinate axis will be 20 rows long.

PWMN, PSMN, Lower limits on bottom-hole pressure, surface pressure, bottom-
TWMN, TSMN, hole temperature, surface temperature and concentration, respec-
CMN tively.

PWMX, PSMX, Upper limits on bottom-hole pressure, surface pressure, bottom-
TWMX, TSMX, hole temperature, surface temperature and concentration, respec-
CMX tively.

READ P-4 (6F10.0)

NOTE: Read as many cards as the observed data points (one card for each value of time at which the observed values are available). Follow the last card with a negative number in the first field specification (F10.0).

LIST: TOX, POW, POS, TOW, TOS, COS

TOX Observation time.

POW Bottom-hole pressure.

POS Surface pressure.

TOW Bottom-hole temperature

TOS Surface temperature.

COS Concentration.

NOTE: The calculated data are read from tape unit 12. If you desire plots for a previous run, tape unit 12 should be attached. If you entered less than NWT sets of the plotting data, follow the last card with a blank card. This is the end of your data set.

MAPS FROM RESTART RECORDS

Restart records may be edited to obtain maps for the dependent variables. The following set of data cards is required to obtain maps for a previous run. Restart records must be available on tape unit 4.

READ M-1 Two title cards.

READ M-2 Control parameters. RSTRT must be non-zero.

READ M-3 This card must be identical to the one used on the original run.

READ M-4 Enter a negative value for TMCHG.

NOTE: Insert as many sets of mapping data (M-5 and M-6) as you desire. Follow the last set with a blank card. The order of times where maps are desired need not be in chronological order.

READ M-5 (I5)

LIST: IMPT

IMPT The time step number at which the maps are desired. A restart record must exist corresponding to this time step (ITIME).

READ M-6 (2I5) (Definition is like READ R1-11 except MAP values should be negative.)

LIST: MAP, MDAT

MAP Requires three digit specification as in READ R2-11, except that it should be negative. Parameter for printing contour maps at time TCHG. Only two-dimensional maps are printed. The maps are printed for r-z coordinates in a radial system and x-y coordinates (areal maps) in a linear system. This parameter requires a three digit specification, the first digit referring to mapping pressures, the second for mapping temperatures, and the third for concentrations.

0 - The variable will not be mapped.

1 - The variable will be mapped at TCHG.

MDAT Control parameter for entering the mapping specifications (see READ R2-11).

0 - The mapping specifications are not to be changed.

1 - Read new mapping specifications. If you are activating the printing of contour maps for the first time during the current run, MDAT must be entered as one.

NOTE: If MDAT has been entered as one, you should enter the mapping data R2-12 through R2-15 at this point.

ERROR DEFINITIONS:

The program checks the input data for a number of possible errors to protect the user from running an entire problem with an error. A detected error will prevent further execution, however the program will continue to read and check remaining data through the last recurrent data set.

If the number of elements in a fixed dimensioned array exceed the dimensions allocated by the main program, you must redimension the array. This requires recompiling the program. The user should refer to the beginning of Appendix D for instructions to redimension the program.

The errors detected in the data input are printed in code numbers in a box. Positions with zeros in the box do not have errors. Errors are defined as follows.

- (1) This error refers to READ M-3. NX is less than or equal to one or NY is less than one or NZ is less than one. The minimum dimensions on the grid block system are 2x1x1. The maximum size is limited only by the available computer storage.
- (3) This error refers to READ R1-1. One or more of CPW and CPR is negative. Physically, heat capacities are always equal to or greater than zero.
- (4) This error refers to READ R1-2. One or more of UKTX, UKTY, ALPHL, ALPHT, and DMEFF is negative.
- (5) This error refers to READ R1-3. Either one or both the fluid densities (BWRN and BWRI) is zero or negative.
- (6) This error refers to READ R1-7 through R1-10. One or more of the viscosity values is entered as zero or negative.

Error numbers 7 through 9 refer to READ M-3.

- (7) HTG is not within the permissible range. HTG is less than 1 or greater than 3.
- (8) The entered value for KOUT is not permissible. KOUT is not equal to 0, 1, or 3.
- (9) PRT exceeded permissible range of -1 to 2.
- (11) This error refers to READ R1-17 through R1-19. One or more grid block sizes (DELX, DELY, DELZ) is zero or negative.
- (12) This error refers to aquifer properties for a homogeneous aquifer (READ R1-20). One or more of the KX, KY, and KZ is negative or PHI is less than 0.001 or greater than 1.0 or SINX or SINY is less than -1 or greater than 1.

- (13) This error refers to heterogeneous aquifer data, READ R1-21. This error applies to both input format options.

I is greater than NX or J is less than 1 or greater than NY or K is less than 1 or greater than NZ or KX or KY or KZ is negative or PHI is less than 0.001 or greater than 1.0.

One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges of 1-NX, 1-NY and 1-NZ respectively, or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.

- (14) This error refers to READ R1-22. The first grid block center (R1) is greater than or equal to the aquifer boundary radius (RE).
- (15) This error refers to READ R1-23. The layer thickness (DELZ) is less than or equal to zero or KYY or KZZ is negative or porosity (POROS) is less than 0.001 or greater than 1.0.
- (16) This error refers to READ R1-24 and R1-25. The sum of NXR's is greater than NX or one or more RER's is greater than RE.
- (17) This error refers to aquifer modifications, READ R1-27. One or more of I1, I2, J1, J2, K1, K2, are out of permissible ranges 1-NX, 1-NY and 1-NZ respectively, or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.
- (18) This error refers to READ R1-28 and R1-29. IAQ is greater than 3 or one or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY and 1-NZ respectively, or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.
- (19) The number of aquifer influence blocks (NABL) are greater than NABLX specified in READ M-3.
- (21) This error refers to READ I-2. One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY and 1-NZ respectively, or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.
- (22) This error refers to READ I-3. One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY, 1-NZ respectively, or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.
- (23) Some of the grid block pore volume is non-zero, and sum of transmissibilities ((cu.ft-cp)/(day-psi)) is zero.
- (24) Some of the grid block pore volume is negative.
- (25) This error refers to READ R2-4. Total number of wells (NWT) is less than 1 or exceeds dimension limit NWMAX.
- (26) This error refers to READ R2-6. Well number I is less than 1 or greater than NWT.

Error numbers 27 through 39 refer to READ R2-7.

- (27) Well location IIW, IWJ is outside aquifer, i.e. IIW is less than 1 or greater than NX or IWJ is less than 1 or greater than NY.
- (28) The well perforations are outside the aquifer, i.e. IIC1 or IIC2 is out of the range 1-NZ or IIC1 is greater than IIC2 or the top block completion interval (K=IIC1) is a zero pore volume block.
- (30) The entered value of IINDW1 is not permissible. The permissible values are +1, +2, and +3.
- (32) A well index of zero is permissible only if IINDW1 is equal to one. This error occurs if IINDW1 is not equal to one and WI is zero or negative.
- (33) IINDW1 is ± 3 and BHP is 0. The specified value of the bottom-hole pressure is a limiting value of the well pressure if IINDW1 is ± 3 .
- (35) All completion layers of a well are in zero pore volume blocks.
- (37) One or more of the KHL values are negative.
- (38) All KHL values are zero for some well. At least one KHL value must be non-zero.
- (39) A well number I is negative or exceeds NWT.
- (40) This error refers to READ R2-2. METHOD is less than -2 or greater than 2 or WTFAC is greater than 1.0.

Error numbers 41 and 42 refer to READ R2-9.

- (41) Minimum number of outer iterations (MINITN) is less than 1 or MINITN is greater than maximum number of outer iterations (MAXITN).
- (42) Method of solution is L2SOR (METHOD = ± 2) and IMPG is less than or equal to zero.

Error numbers 43 through 46 refer to READ R2-10 and R2-11.

- (43) The time at which next set of recurrent data is to be entered (TCHG) is less than or equal to current TIME.
- (44) DT is zero for the first time step. Automatic time step control may not be initiated until at least the second time step.
- (45) DTMAX is less than DTMIN.
- (46) The value entered for MAP is not permissible. All three digits must be 0 or 1.

Error numbers 47, 48, and 49 refer to READ R2-13, R2-14, and R2-15 respectively.

- (47) IP2 is greater than NX or KP2 is greater than NZ or HTG is not equal to 3 and JP2 is greater than NY.
- (48) IT2 is greater than NX or KT2 is greater than NZ or HTG is not equal to 3 and JT2 is greater than NY.
- (49) IK2 is greater than NX or KK2 is greater than NZ or HTG is not equal to 3 and JK2 is greater than NY.