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# Water Property Lookup Table (SANWAT) For Use With the Two-Phase Computational Code Shaft

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WATER PROPERTY LOOKUP TABLE (SANWAT) FOR  
USE WITH THE TWO-PHASE COMPUTATIONAL CODE SHAFT

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ABSTRACT

A lookup table for water thermodynamic and transport properties (SANWAT) has been constructed for use with the two-phase computational code, SHAFT. The table, which uses density and specific internal energy as independent variables, covers the liquid, two-phase, and vapor regions. The liquid properties of water are contained in a separate subtable in order to obtain high accuracy for this nearly incompressible region that is frequently encountered in studies of the characteristics of nuclear-waste repositories.

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## Nomenclature

		<u>Units</u>
DB	Density (table ordinate)	$\text{kg/m}^3$
DDS	Saturation density for a given energy	$\text{kg/m}^3$
DF	Saturation liquid density	$\text{kg/m}^3$
DG	Saturation vapor density	$\text{kg/m}^3$
DSAT	Saturation density for given energy	$\text{kg/m}^3$
DX	Density from equation solution	-
e	Specific internal energy	-
EB	Energy (table abscissa)	-
EDS or ESD	Saturation energy for a given density	-
EF	Saturation liquid energy	-
EG	Saturation vapor energy	-
EX	Energy from equation solution	-
NDLOK	Defined such that $E(\text{NELOK}) < EX < E(\text{NELOK}+1)$	-
P	Pressure	pascals
T	Temperature	$^{\circ}\text{C}$
TSATR	ub-energy (table abscissa)	-
X	Quality	-
$\rho$	Fluid density	$\text{kg/m}^3$



WATER PROPERTY LOOKUP TABLE (SANWAT) FOR  
USE WITH THE TWO-PHASE COMPUTATIONAL CODE SHAFT

Introduction

The two-phase code SHAFT<sup>1</sup> solves for energy,  $e$ , from the conservation-of-energy equation and density,  $\rho$ , using the conservation-of-mass equation (see Figure 1). Consequently, it is necessary to have an equation-of-state lookup table for water that relates  $(e, \rho)$  to temperature ( $T$ ), pressure ( $P$ ), and saturation ( $S$ ). Available source materials such as the 1967 American Society of Mechanical Engineers (ASME) Steam Tables<sup>2</sup> use  $(T, P)$  as independent variables. It is therefore required to map  $(T, P)$  into the  $(e, \rho)$  field. This report details an appropriate mapping procedure.

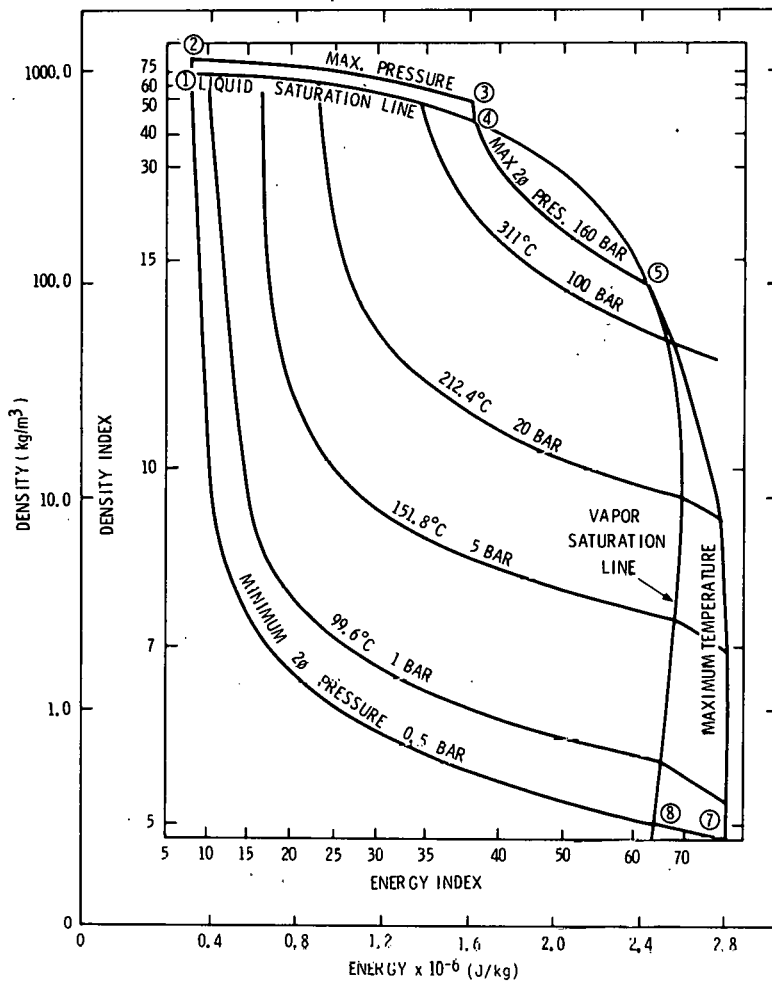


Figure 1. Water Properties

An equation-of-state lookup table for water was originally constructed at Lawrence Berkeley Laboratory (LBL) for use in the SHAFT 78 computer code. LBL developed SHAFT<sup>1</sup> in order to study certain geothermal problems of heat and mass transfer through porous rock. These problems focused on the process of water boiling and steam condensation in geothermal applications involving the exchange of large quantities of heat between the fluid and the rock matrix. Sandia National Laboratories then modified the LBL table so that SHAFT could be used to study nuclear-waste disposal problems. The table was divided into two subtables--one for the liquid region and one for the two-phase vapor region. This extension was required to obtain the table lookup accuracy needed in the liquid region over a large pressure range (up to 900 bar) and at a wide temperature range extending down to 10°C.

Using density and energy as independent variables has two advantages: (1) The two variables are independent even in the two-phase region, and (2) They are the natural variables arising in the conservation forms for the energy and mass-flow equations. However, the use of  $\rho$  and  $e$  introduces several problems. The main problem is how to accurately determine the liquid water pressure. In the nearly incompressible liquid region, because small changes in liquid density at constant energy correspond to large changes in pressure, accurate interpolation within the tables must be done. Therefore, Sandia has developed a method of table formation based on the use of a separate liquid subtable that is felt to be more accurate than the method developed at LLB. The table for the vapor and two-phase (2 $\phi$ ) regions remains similar to that used by LBL.

#### Construction of "Main" Table

Figure 1 shows a schematic plot of water properties that uses density (log ordinate) and energy (abscissa) coordinates. The second set of coordinates shows a typical spacing of the density and energy index numbers used in the lookup table. The "main" table, which covers the 2 $\phi$  and vapor region, uses 81 energy subdivisions and 74 density subdivisions. The interval locations (DB and EB) from which the table is constructed must be obtained by using good judgment.

Because the thermodynamic derivatives are discontinuous across the saturation line, interpolation across this line must be avoided. In our first computer program, TVALUES, we specify a set of temperature values and compute the corresponding pressures, energies, and densities along the liquid saturation line between Points (1) and (4) (see Figure 1).\* We then specify a second set of temperatures and compute the pressure, energies, and density along the vapor saturation line, Points (5) to (8). The region between Points (4) and (5) is filled in with intermediate values of energy and density. Since we are interested only in 2 $\phi$  and vapor pressures up

---

\* Values of temperature, not energy or density, are specified on the saturation line because most equation-of-state water routines use temperature as the independent variable. Also, most problems are usually defined in terms of temperature and pressure limits.

to 160 bar, no attempt is made to define the saturation line near the critical point. The intermediate range ((4) to (5)) was filled in with evenly spaced values at energy and density.

In addition, several values of energy were selected to the right of the vapor saturation line to define the vapor region, up to the maximum specified temperature. Note that the slope of the saturation line in  $\rho - e$  coordinates is negative for densities above about  $15 \text{ kg/m}^3$ ; for smaller densities the slope becomes positive. This means that the resulting (e) values along the vapor saturation line are not monotonically decreasing with increasing density. Some shifting of the density-energy combination must be made in this region for the double-valued function. That is,  $\text{DDS}_3$  must equal  $\text{DDS}_4$  (see Figure 2). In code TVALUES, the 74 values of energy and

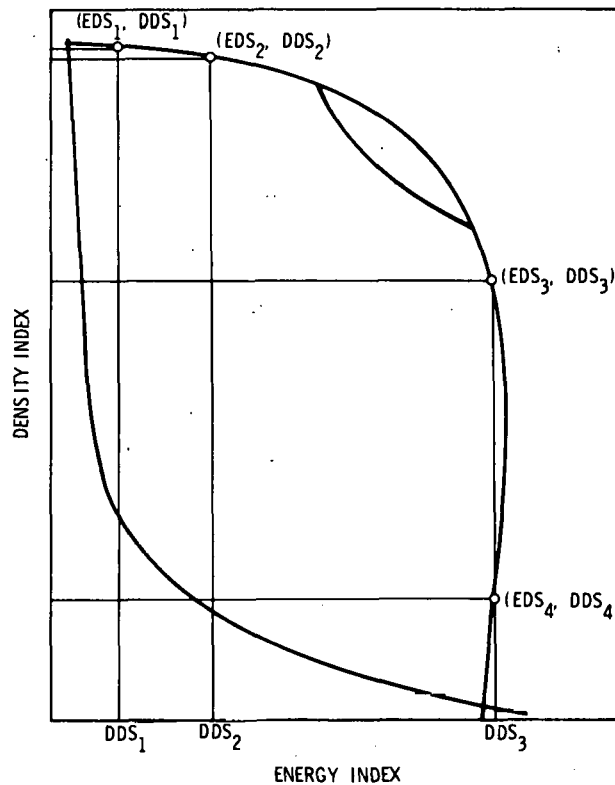


Figure 2. Typical (EDS, DDS) Pairs That Must Coincide with Saturation Line

densities are reshuffled to ensure that both the EB and DB arrays are monotonic. In summary, we now have 58 EB and DB coordinate locations located on the saturation line and 13 additional EB, DB points covering the maximum temperature vapor region, (Figure 3). The first 10 low-energy points are reserved for low-energy liquid water, (see Liquid, Table A).

Our second computer program, MAIN, constructs the final table in four stages, given the EB and DB array shown in Figure 3. A full set of water properties will be calculated for each EB, DB coordinate point lying within the pressure temperature range specified ( $2\phi$  and vapor only).

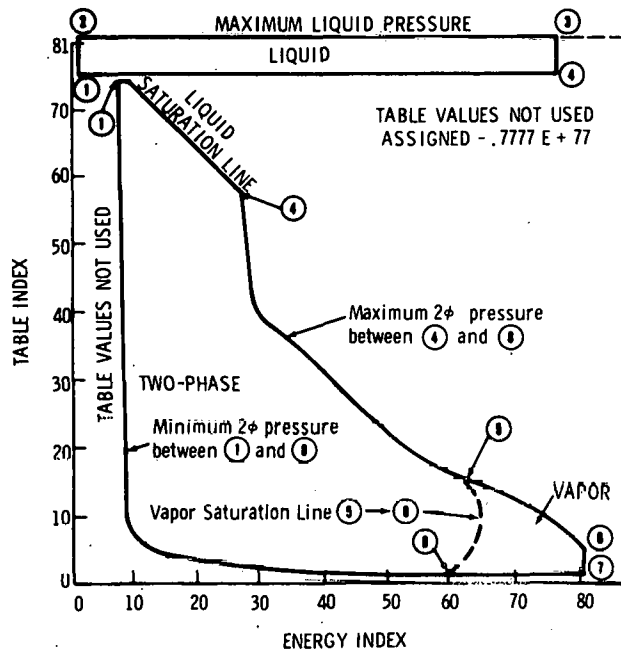


Figure 3. Energy-Density Pressure Matrix of Table Points

A list of the four steps executed by the code MAIN is given below, followed by a detailed explanation of each step.

1. Form a pressure-energy table by using density and temperature and phase of each point.
2. Form preliminary density-energy table. Obtain temperature and pressure by linear interpolation.
3. Use two dimensional Newton-Raphson formula to obtain accurate temperature and pressure values.
4. Use temperature and pressure values to obtain remaining water properties.

#### Step 1

The pressure-energy table is formed by first determining values of density and temperature at each point. The lowest pressure value and the increment of pressure are input. For each pressure value the corresponding saturation temperature is computed by using subroutine TSAT. Then the saturated liquid energy and saturated vapor energy for each pressure are computed. The phase of a given pressure-energy point is determined by comparing the value of energy with the saturation energy values: the point is in the liquid region if the energy is below the saturated liquid energy, in the vapor region if the energy is above the saturated vapor energy, and in the 2 $\phi$  region if the energy lies between the two values. The liquid points are considered during construction of the liquid subtable.

For the single vapor-phase region, the temperature is estimated from an approximate relation of the form  $T = T(e)$ . Accurate temperature values are obtained by Newton-Raphson iteration of an accurate relation of the form  $e = e(T,P)$  for

given P. With the temperature and pressure known, the density is obtained from a relation of the form  $\rho = \rho(T,P)$ .

#### Step 2

The second step in the program is the preliminary formation of a density-energy table. At each energy, for a given density value, DB, the pressure values that bracket the density value are found in the pressure-energy table. The pressure-energy table is then interpolated to obtain approximate values of pressure and temperature for points on the density-energy table.

#### Step 3

To get accurate values of temperature and pressure, the third stage of the program uses a two-dimensional Newton-Raphson formula to solve two relations of the form  $e = e(T,P)$  and  $\rho = \rho(T,P)$  iteratively until the absolute value of the changes in temperature and pressure are  $10^{-5}$ °C and  $10^{-3}$  Pa. Partial derivatives are approximated by finite differences. The following are computed in the  $2\phi$  region for a given approximate temperature: (1) the corresponding saturation pressure; (2) liquid saturation energy (UF) and density (DF); and (3) vapor saturation energy (UG) and density (DG). The corresponding quality for a given density is then computed. Using this value of quality, the mixture energy is computed and compared to the required value. The temperature is obtained by Newton-Raphson iteration until the discrepancy in energy is less than  $10^{-8}$  J/kg.

#### Step 4

In the fourth step, the temperature and pressure at each point on the density-energy table are taken and are used to compute

- Temperature
- Pressure
- Saturation (volume fraction of vapor)
- Thermal conductivity
- Liquid relative permeability/liquid viscosity
- Vapor relative permeability/vapor viscosity
- Liquid density
- Vapor density
- Liquid energy
- Vapor energy

#### New Liquid Subtable

The increase in pressure with increased density at constant energy is so large in the liquid region that the liquid regime occupies a very narrow band above the liquid saturation line and becomes even narrower at lower energy, where water is more nearly incompressible (see Figure 4). In LBL SHAFT, water properties are linearly interpolated between three points--two on the saturation line and one at the intersection of the constant density and energy lines, shown as Point 3 in

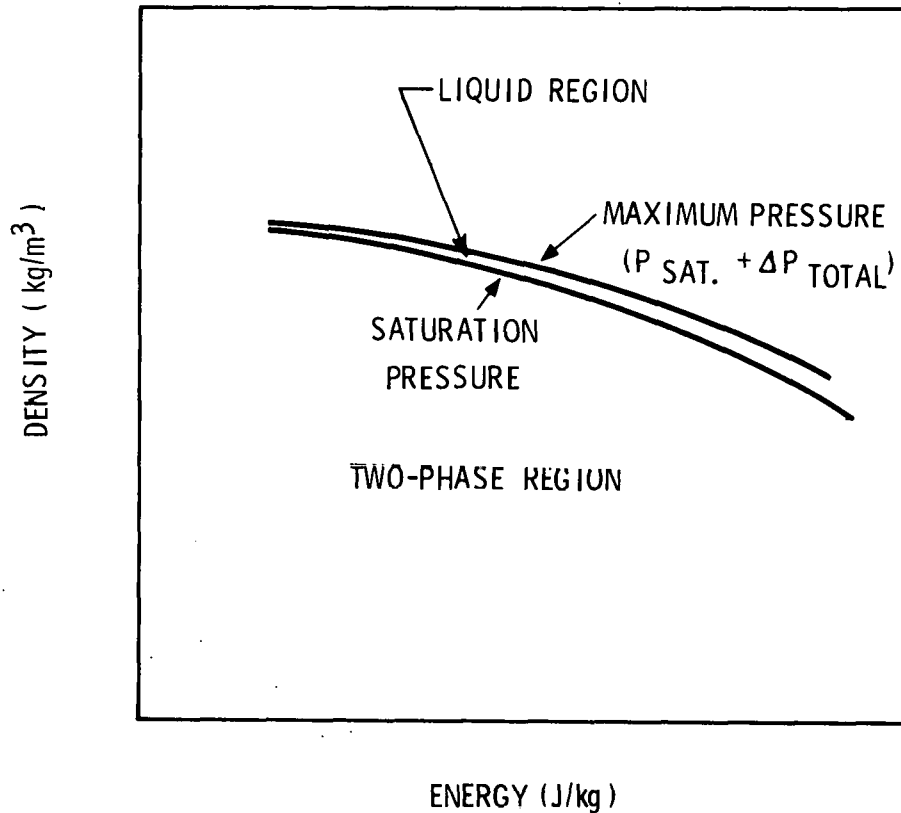


Figure 4. Definition of Liquid Water Region

Figure 5. This point will usually be at high pressure. Accuracy is difficult to obtain because LBL considers the liquid water properties as an integral part of the main table. The maximum error in pressure in the LBL table is 6%, with a total pressure range of less than 10 bars. For the Sandia nuclear-waste problem, with its considerably greater ranges of pressure and temperature, the results would be worse. Consequently, the water properties are constructed as a separate subtable. Details of this development follow.

#### Sandia Liquid Subtable A

The idea of using a density-energy table in the liquid region has been abandoned. Lines corresponding to Densities 75 to 81 are used for the liquid table. On table Line 75, each point corresponds to liquid saturation at a given energy. The pressures corresponding to the points on Line 76 are above saturation pressure by a specified pressure increment ( $\Delta P$ ); those on Line 77 are above saturation by  $2\Delta P$ , etc. (see Figure 6). The temperature is obtained by a Newton-Raphson solution of  $E = E(P,T)$ . Knowing  $P$  and  $T$ , we can easily obtain density and all other transport properties.

Use of this table ensured that reasonably accurate results were obtained when pressures for problems of interest were in a narrow range of 1 to 9 bars. When higher pressures became of interest, the same method was used, except that the new liquid table contained much larger pressure increments ( $\Delta P$ ) between table lines.

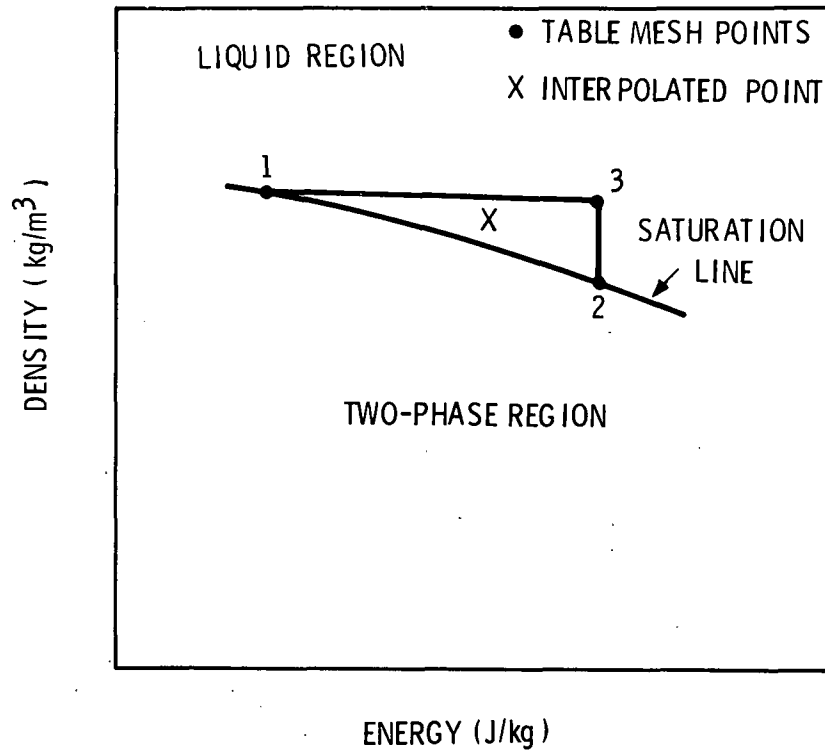


Figure 5. Interpolation for Points in Liquid Region

These tables, although better than the original LBL table, were not always satisfactory. As a result, further changes discussed in the next section were made.

#### Sandia Liquid Subtable B

Much wasted memory results from using density and energy as independent variables in the table (see Figure 3). Many points in the rectangular  $\rho - e$  grid correspond to pressures and/or temperatures that are too high or too low. As a result, more than half of the water table is filled with the default number  $-0.7777E177$  for all 10 entries at the point. One way to increase accuracy and eliminate some of this waste of memory is to use different energy steps in the liquid and  $2\phi$  regions.

For the liquid region, maximum energy corresponds to less than half the number of energy points (40 out of 81). It was realized that the energy points in the liquid table did not have to agree with those in the main table. Each energy increment in the main table was therefore cut in half. This means that if energy EX is between points NELOK and NELOK+1 in the main table, it will be between points  $2*NELOK-1$  and  $2*NELOK$  or between  $2*NELOK$  and  $2*NELOK+1$  in the liquid table. This results in nearly full use of all the points in the liquid table. Halving the energy increment greatly increases the accuracy of the pressure determination. The worst errors are 0.2% of the absolute pressure, about 1.9 bar, for  $p_{max} = 900$  bar. This improvement is to be expected because the error in quadratic interpolation

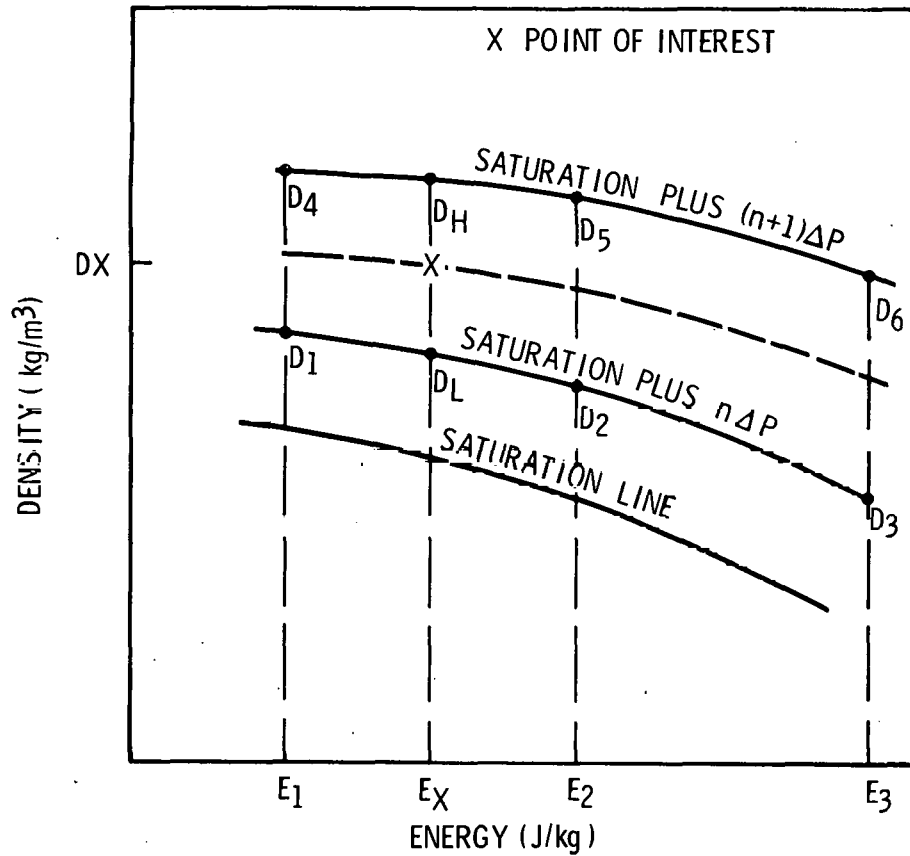


Figure 6. Data Used for Interpolation Scheme

should be approximately proportional to the cube of the energy increment. (Halving the increment cuts the interpolation error in the energy direction by about one eighth.)

The accuracy of the liquid pressure and temperature computation has been tested in a test program. Pressure and temperature are input, and the corresponding liquid energy and density are computed. These values are input into the subroutine GETIT that performs the interpolation. The resultant pressure and temperature coming from the tables are output. The errors as a function of the fractional distance from the lower density-energy point were compared. Only very small errors are expected near any of the points (zero error at the points) and maximum errors near the middle of the interpolation region. Temperature errors are typically less than 0.01%.

#### Incorporation of SANWAT into SHAFT

Because the basic construction of SANWAT differs appreciably from that of the original LBL table, many program changes were necessary to make the new table compatible with SHAFT 78. These changes were limited to subroutine GETIT.



Subroutine GETIT is entered with energy EX and density DX. GETIT locates EX between energies E1 and E2. The fractional distance of EX between E1 and E2, Q, is obtained linearly by using Eq. 1:

$$Q = \frac{EX - E1}{E2 - E1} \quad (1)$$

GETIT contains logic to determine whether or not the point of interest is in the main or the liquid table. In the main table, the fractional distance of DX between the bounding densities D1 and D2, P, is obtained by linear interpolation

$$P = \frac{DX - D1}{D2 - D1} \quad (2)$$

For the liquid table, the density DL shown on Figure 6 is obtained by quadratic interpolation, using densities D1, D2 and D3. Density DH is likewise found, using D4, D5 and D6. Quadratic rather than linear interpolation is used because

$$\left(\frac{\partial P}{\partial e}\right)_{[P_{sat} + n\Delta P]} \quad (3)$$

is highly nonlinear. The fractional distance between DL and DH, P, is obtained by linear interpolation

$$P = \frac{DX - DL}{DH - DL} \quad (4)$$

Linear interpolation can be used because

$$\left(\frac{\partial \rho}{\partial P}\right)_e \cong \text{constant} \quad (5)$$

The rest of the properties (page 11) are obtained from P and Q by double linear interpolation.

The current version of subroutine GETIT (Appendix A) has been tested by computing the water and geologic properties about a heat-generating waste canister. The geologic medium at time = 0 was cold (temperature = 28°C). As time progressed, the water in the pores went from 1φ liquid to 2φ, and finally to vapor. No difficulties were incurred in crossing the saturation curve that separates the regions.

#### References

<sup>1</sup>K. Pruess et al, SHAFT78--A Two-Phase Multidimensional Computer Program for Geothermal Reservoir Simulation, LBL-8264 (Berkeley, CA: Lawrence Berkeley Laboratory, Earth Sciences Division, January 1979).

<sup>2</sup>C. A. Mayer et al, "Thermodynamic and Transport Properties of Steam," The American Society of Mechanical Engineers, 1967.

## APPENDIX A

### Subroutine GETIT

The flow diagram of the revised subroutine GETIT is given by Figure A-1. This is provided to show the revisions required to the original GETIT to make GETIT compatible with SANWAT, which contains the separate liquid subtable. A nomenclature list for the symbols used in the flow chart is given below.

#### Flow-Chart Nomenclature

DSAT	Saturation density for given energy
DB	Density (table ordinate)
DX	Density from equation solution
EB	Energy (table abscissa)
E2	Energy from table
Key C	Time-step counter
NDLOK	Defined such that $D(NDLOK) < DX < D(NDLOK+1)$
NE	Maximum table index for energy
NELOK	Defined such that $E(NDLOK) < EX < E(NELOK+1)$
P	Fractional distance $(D_X - D_L)/(D_H - D_L)$ (See Figure 6)
Q	Fractional distance $(EX - E1)/(E2 - E1)$ (See Figure 6)
$\rho$	Density
$\phi$	Phase
Subscripts	
l	Liquid
u	Energy



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