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A PROPOSAL OF STEAM TABLE INCLUDING METASTABLE STATES

July 1983

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A PROPOSAL OF STEAM TABLE INCLUDING METASTABLE STATES

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Steam tables have been produced in which the physical properties of water are available not only in the stable states, but also in the metastable states. The properties of water in the metastable states have been obtained by extrapolating the IFC formulation into the metastable regions. Two steam tables have been generated for each phase. The steam tables contain the thermodynamic properties such as temperature, pressure, specific volume, specific internal energy, specific enthalpy, coefficient of thermal expansion, isothermal compressibility and heat capacity at constant pressure. The tabular data are used to determine other thermodynamic properties using input data of pressure and enthalpy for each phase. For this determination the STH2O program which is used in the RELAP4 code has been improved to be able to calculate the properties of both stable and metastable states. Although the metastable regions obtained by the extrapolations are limited, the metastability limits from our calculations are comparable to the maximum liquid superheat and maximum vapor supercooling which have been obtained by the experiments and to the spinodal lines of van der Waals fluids.

Keywords: Steam Table, Metastable, IFC Formulation, Metastability Limit
Superheat, Supercooling, Spinodal Line, STH2O Program

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* On leave from Japan Information Survice, Ltd.

準安定状態を含む蒸気表の提唱

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（1983年7月4日受理）

安定状態と準安定状態の水の物理量を含む蒸気表が作成された。準安定状態の水の特性は，IFCの式を準安定領域に外挿して得られた。各々の相に対応する2つの蒸気表が作成された。蒸気表は，温度，圧力，比体積，比内部エネルギー，比エンタルピー，熱膨張係数，定温圧縮率及び定圧比熱の熱力学諸量を含む。各相の圧力とエンタルピーを入力データとして，他の熱力学諸量を決定するために，この表は使用される。この決定の際，安定状態と準安定状態の量を計算できるように，PELAP4コードで使われているSTH2Oサブルーチンパッケージを改良した。外挿で得られた準安定領域には限界があるが，我々の計算で得られた準安定の限界は，実験で得られている水の最大過熱や蒸気の最大過冷却やファンデアワールス流体のスピノーダル線と比較して妥当な領域にある。

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* 業務協力員；日本情報サービス㈱

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1. Introduction

"Steam Table" is one of the most fundamental data of water to analyze postulated light water reactor accidents. During the last several decades a great deal of research concerning the thermodynamic properties of water has been carried out in many countries. From 1925 to 1967 six international steam table conferences have been held in order to analyze the existing experimental data and investigate the empirical thermodynamic relations of steam. The 1967 International Formulation Committee (IFC) formulation (1967 ASME Steam Table)[1] is the most accurate equation of state for water until now. The formulation is suitable to the stable liquid and vapor states.

Thermodynamic processes in transient two-phase flow phenomena such as flashing[2] often lead to metastable states of water in which liquid can be suddenly superheated or vapor subcooled. Existing knowledge of physical properties of water is limited in the metastable states. The formulations in the metastable region still remains under investigation in many countries. F. Bakhtar and M. Piran[3] have given an equation of state for the supercooled vapor by applying the virial equation of state by Vukalovich and the distribution functions describing the concentration of the molecular clusters which is obtained by nucleation theory. They have compared a number of properties of water obtained from the equations using second virial coefficient alone and the equations used by Keenan, Keyes, Hill and Moore (KKHM) and Vukalovich. The differences among them are considerable for C_p and κ. For specific enthalpy and specific volume the differences are relatively small.

A. Karimi and J. Lienhard[4] have somehow simplified the KKHM fundamental equations for water to satisfy the Maxwell constraint. They have used the equations in the region of the metastable states by extending the thermodynamic properties beyond the saturation line. The KKHM equations of state are, however, obtained by fitting not to the caloric data such as β, κ and C_p, but only to the stable liquid P-v-T data. It may not be suitable, therefore, to use the KKHM equations in the computer code for reactor safety analysis.

Recently some advanced codes have been developed to have unequal temperature models. The models can predict the thermodynamic states of water such as supercooled, superheated, saturated liquid or vapor. (Fig.1) Each code

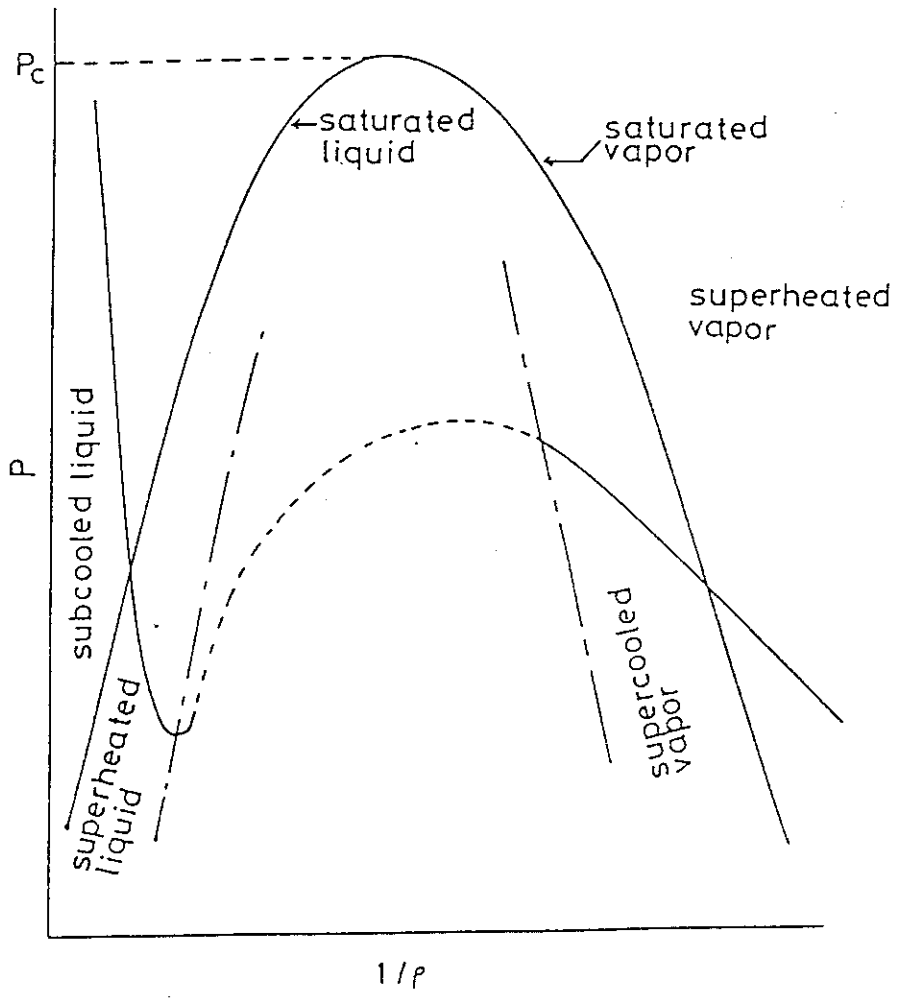


Fig. 1 Thermodynamic States of Water in Pressure-Volume Diagram

considers the equations of state in the metastable states in each way. In the RELAP5 code[5] the properties in the metastable states are taken by extrapolating linearly quantities at saturation along isobars. The properties of C_p, κ and β in the metastable states are assumed to be evaluated at saturation. In the TRAC computer code[6], the thermodynamic properties are calculated by the simplified polynomials. The polynomials are obtained by fitting to the ASME steam table and used in the wide range of the stable and metastable states. The equations used in TRAC provide a fast computation but are so simple compared to the IFC formulation.

We have tried to improve the above problem by using the accurate ASME steam table and calculating the properties of C_p, κ and β in the metastable regions. We will show it in this paper. The tables of thermodynamic properties of water which cover the stable and metastable states have been generated by means of extrapolating the equations of state of the IFC formulations into the metastable regions. The extrapolations have been performed by extending the thermodynamic properties beyond the saturation line. The generated steam tables are used to calculate other thermodynamic properties using input data of pressure and enthalpy. We have extended the subroutine "STH2O5" in the "STH2O" program[7] used in the RELAP4 code so as to be able to estimate the thermodynamic properties in the metastable states. In our steam tables three data libraries are available. Three correspond to the original steam table, the steam table for the vapor state and that for the liquid state.

We will present how to produce the steam tables including the thermodynamic properties in the metastable states in Section 2. In Section 3 the improvement of the STH2O program will be described. The usage of the improved subroutines will be presented in Section 4.

2. GENERATION OF STEAM TABLES INCLUDING METASTABLE STATES

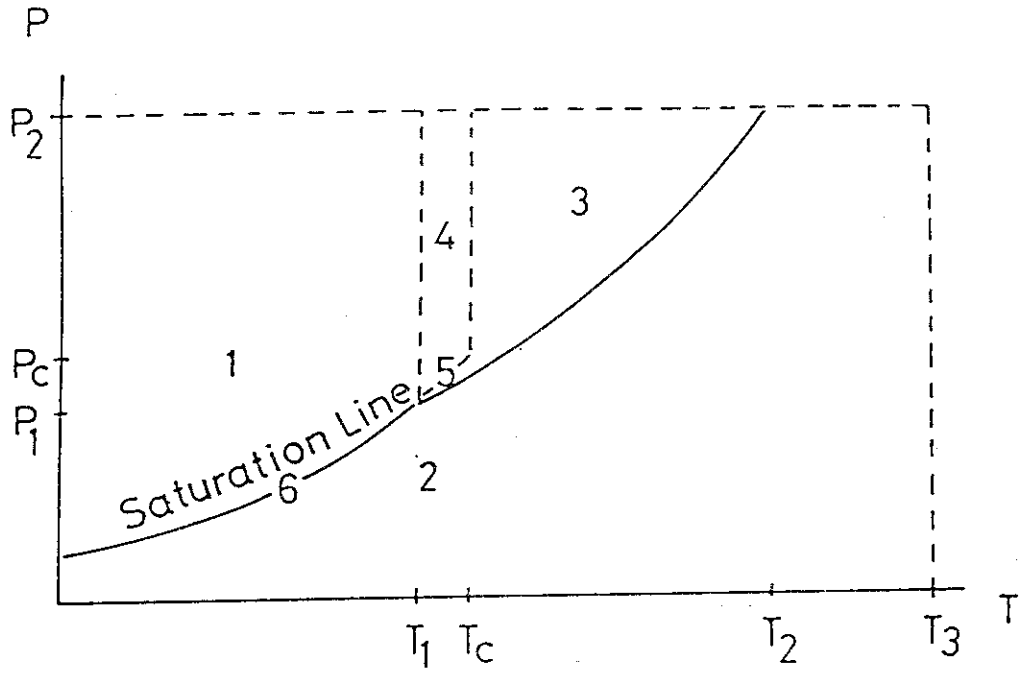
The expressions for all thermodynamic properties in the IFC formulation are derived directly by partial differentiation of the canonical functions, Gibbs and Helmholtz functions, and maintain thermodynamic consistency.[1] The formulation is coded in the subroutine library "STEAM"[8] in JSSL (JAERI Scientific Subroutine Library)[9]. The formulation presented describes the thermodynamic properties of water in the region that covers in pressure from zero to 10^8 N/m^2 (1.02×10^3 kg.f/cm^2) and in temperature from 273.16 K (0.01 °C) to 1073.15 K (800 °C). The generation of steam tables including the metastable states have been performed by extending the IFC formulation beyond the saturation line into the metastable regions. The calculation scheme for each steam table by using the subroutine "STEAM" is presented in Appendix 1. It is assumed in this extrapolations that all thermodynamic relations used in the stable states are satisfied in the metastable states(see Appendix 4).

The whole region in the pressure-temperature diagram of the ASME steam table is divided into six regions which are shown in Fig.2. The different subroutines in "STEAM" are used in dependence on the regions. The names of these subroutines are shown in the following list. The original array AA(I) shows the steam table which is produced by the original subroutine "STEAM". Metastable values of the thermodynamic properties have been obtained by means of changing the subroutines in each region in "STEAM" as follows:

Steam Table	AA(I)	BB(I)	CC(I)
Subregion 1	SUB1	SUB2	SUB1
Subregion 2	SUB2	SUB2	SUB1 (see note)
Subregion 3	SUB3	SUB3	SUB4
Subregion 4	SUB4	SUB3	SUB4

(note: SUB4 between $T_t/T_c < T/T_c < 1.0$)

The array BB(I) presents the steam table of vapor including the supercooled state. The array CC(I) is that of liquid having the superheated state.



T_1 = 623.15 K $\quad P_1 = 1.654 \times 10^7$ N/m^2

T_2 = 863.15 K $\quad P_2 = 1.000 \times 10^8$ N/m^2

T_3 = 1073.15 K $\quad P_c = 2.212 \times 10^7$ N/m^2

T_c = 647.3 K

Fig. 2 Subregions of ASME Pressure-Temperature Diagram

The extrapolations of the IFC formulation lead to bad behaviors such as negative values of volume, enthalpy or heat capacity, if they are carried out much beyond the saturation line. We have stopped performing the extrapolations before such behaviors start to occur. Figure 3 shows the region of metastable states in the pressure-temperature diagram for the state of water. The formulations cover the wide range in the metastable state except for the region near the critical point. The lines, P_{b_1} (T) or T_{b_1} (P) and P_{b_2} (T) or T_{b_2} (P) describe the maximum vapor supercooling and the maximum liquid superheat which have been obtained in our calculations. The line equations for the metastablility limits are shown in Appendix 2.

We show in Fig.4 the line equations of the obtained metastability limits, T_{b_1}/T_c and T_{b_2}/T_c, as a function of reduced saturation temperature, T_{rs}. We will compare these lines to the existing lines of the maximum vapor supercooling and the maximum liquid superheat which are given by correlating the experimental results.

The maximum liquid superheat and the maximum vapor supercooling of fluids have been studied for the last two decades by many investigators. Recently J. H. Lienhard's group has intensively made an investigation of these themes. They have obtained a correlation line for the limiting liquid superheat from the data of Skripov for 12 substances[10),11),12)], which will be referred as Lienhard's correlation in Fig.4, as follows.[13),14),15)]

$$T_{rM} - T_{rs} = 0.905 - T_{rs} + 0.095\, T_{rs}^{8}$$

where T_{rM} is the maximum reduced superheat temperature and T_{rs} is the reduced saturation temperature at a given pressure. They have also attempted to represent P – v – T surfaces with van der Waals' classic equation of state.

$$P_r = 8\, T_r/(3v_r - 1) - 3/v_r^2$$

The liquid and vapor spinodal lines of a van der Waals fluid, which are the lines of the maximum liquid superheat and the maximum vapor supercooling, can be given by combining the last equation with

$$T_{rsp} = (3v_r - 1)^2/4v_r^2$$

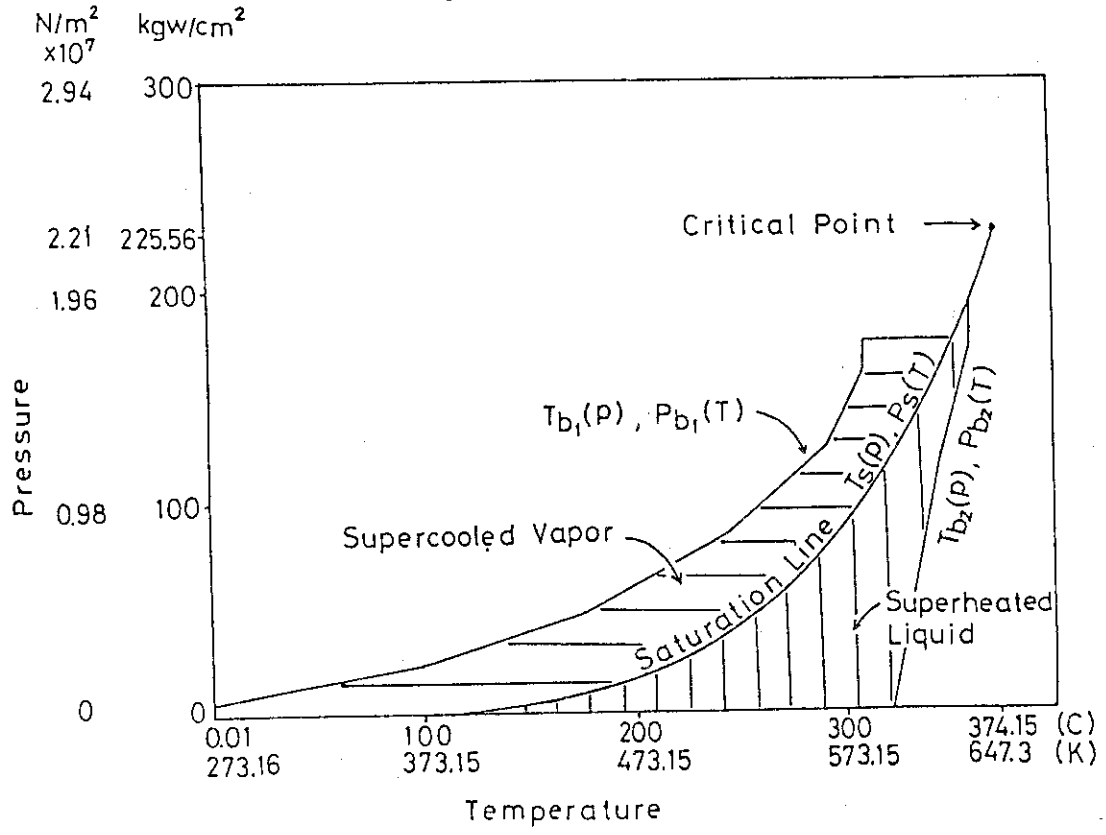


Fig. 3 Metastable Regions in Pressure-Temperature Diagram

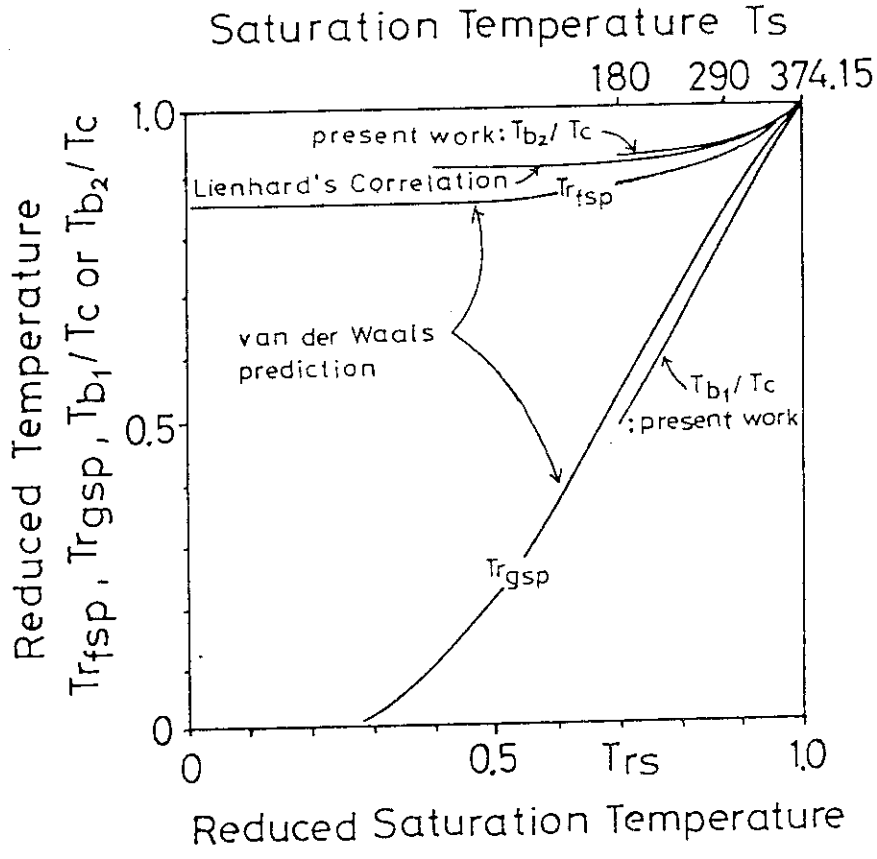
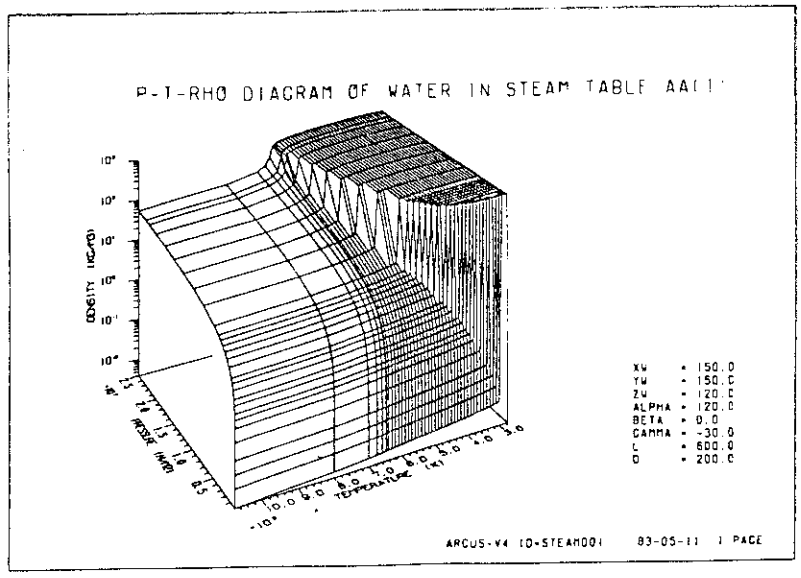


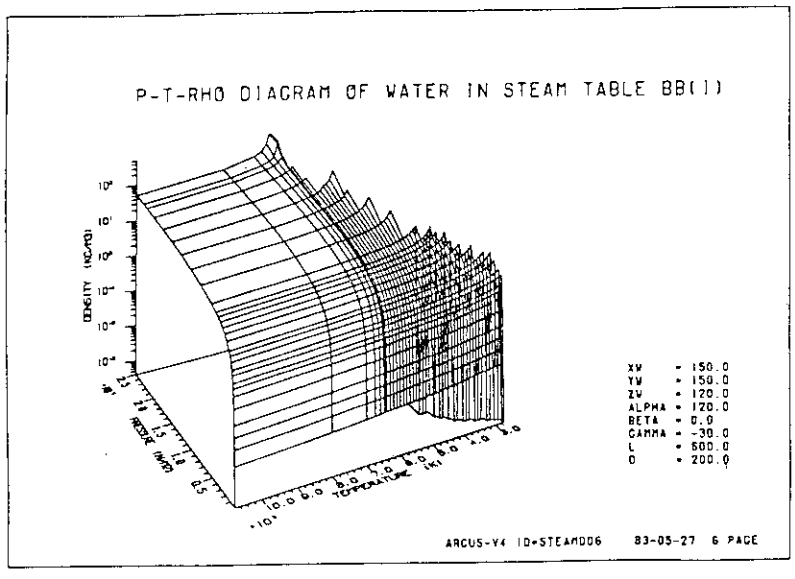
Fig. 4 Comparison of Maximum Liquid Superheats and Maximum Vapor Supercoolings

As for the limiting vapor supercooling the measurements of the vapor nucleation temperature have been made in nozzle[16),17),18)] and shock tubes tests[19)] and diffusion cloud chambers.[20)] It is shown that the data for the nucleation temperature deviate much farther from the van der Waals' prediction toward the saturation line. In Fig. 4 , are shown the liquid and vapor spinodal temperatures, T_{rfsp} and T_{rgsp}, as a function of T_{rs}. As can be seen in the figure, the metastability limits obtained from the IFC formulation lie in the region enough to cover the existing metastability limits from the experimental results.

The storage of each table is shown in Appendix 4. The original steam table is stored in the array AA(I). The array BB(I) is a steam table for the vapor state and contains the properties at P_{b_1} (T) or T_{b_1} (P) instead of liquid properties at P_s (T) or T_s (P) in the original steam table. The array CC(I) is a steam table for the liquid state and includes the properties at P_{b_2} (T) or T_{b_2} (P) instead of vapor properties at P_s or T_s in the original steam table.

The physical properties which were obtained in our calculations are sketched as a function of two independent variables, pressure and temperature, in Figures 5-1 through 5-5. In these figures meshes of coordinate axes for pressure and temperature have been used in the same way as in RELAP4[7)] .





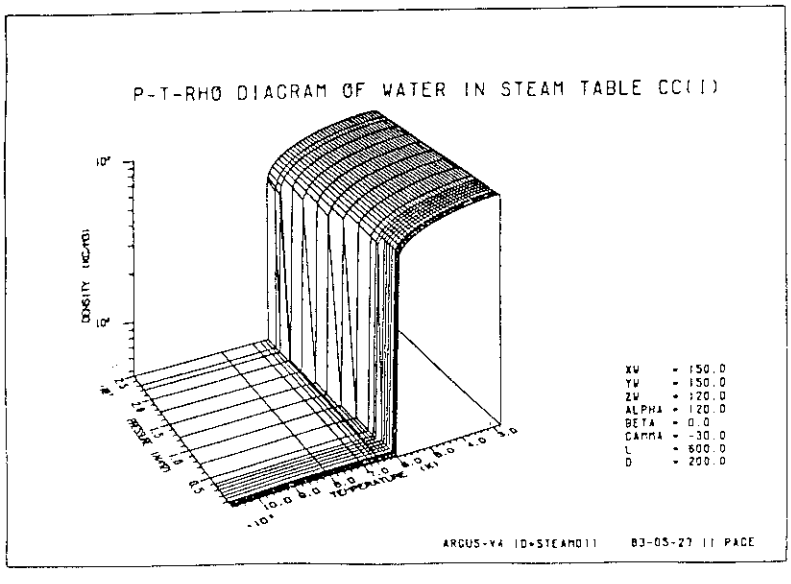
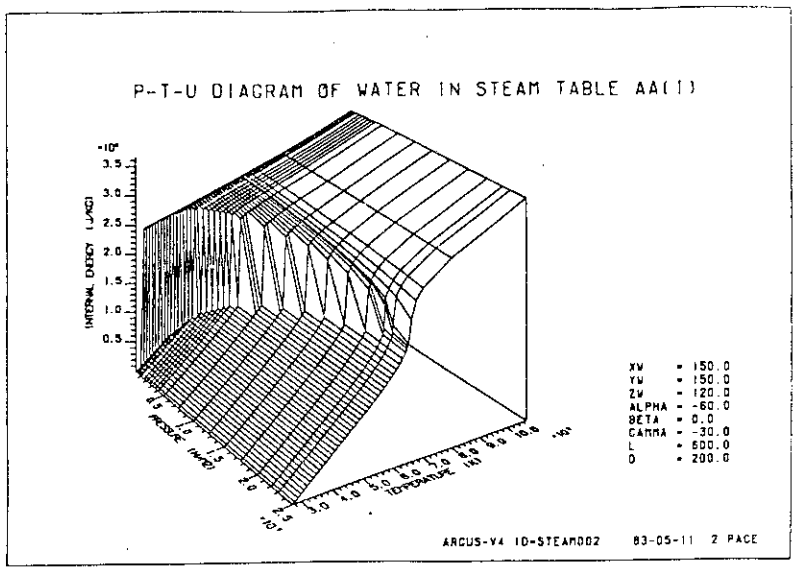
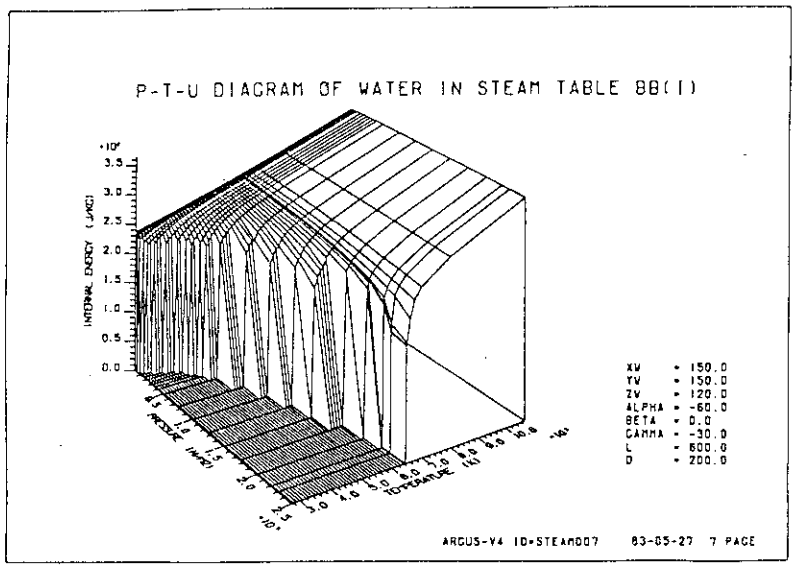


Fig. 5-1 P-T-1/v Diagram of Steam Tables





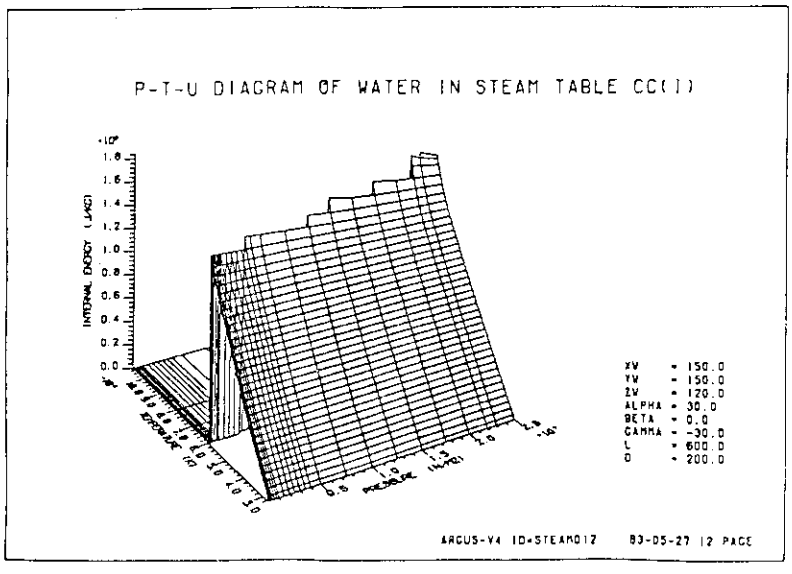
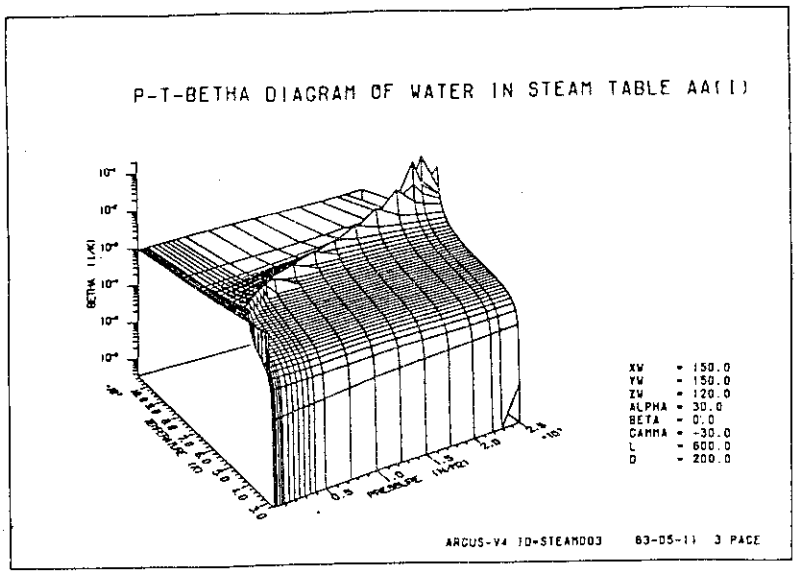
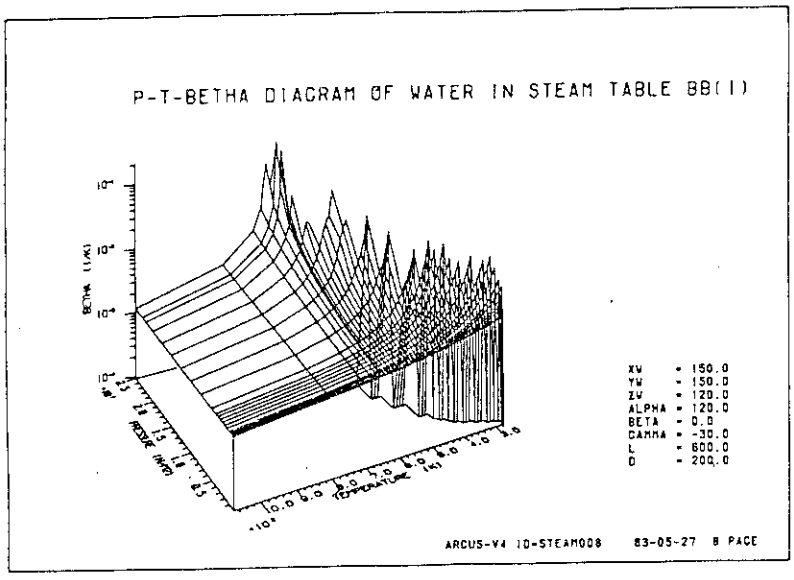


FIg. 5-2 P-T-u Diagram of Steam Tables





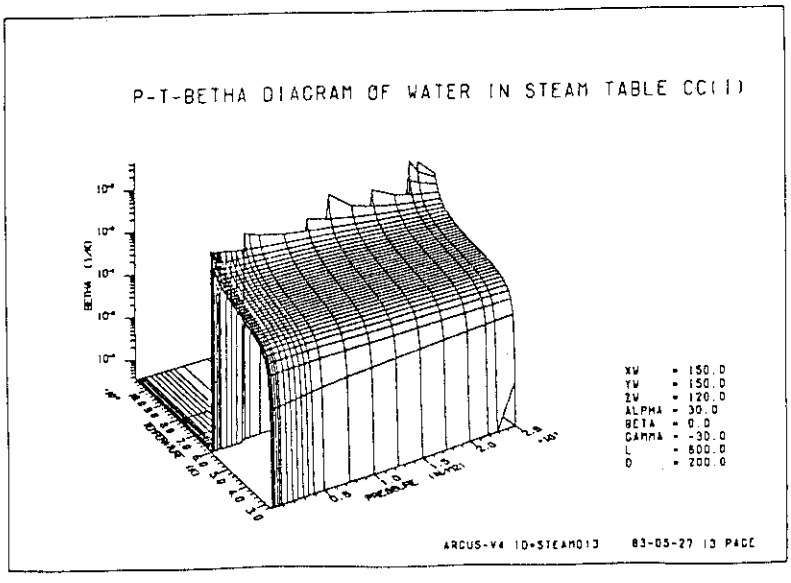
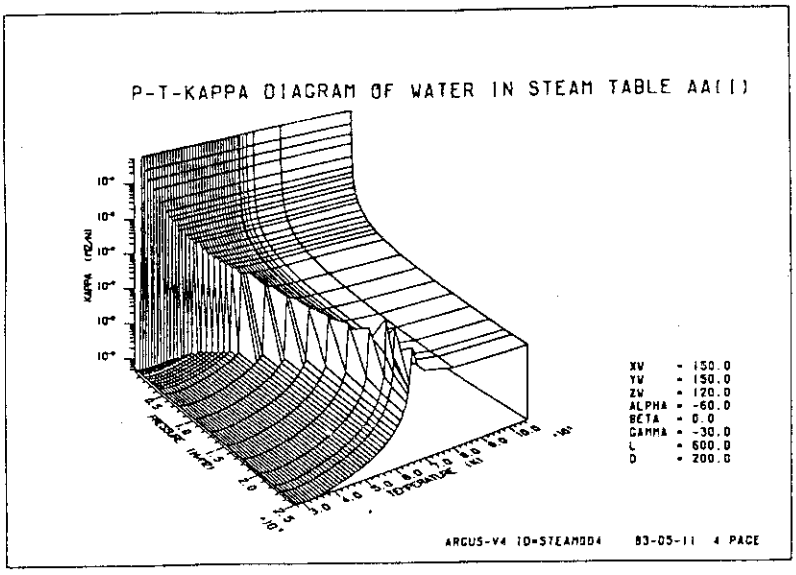
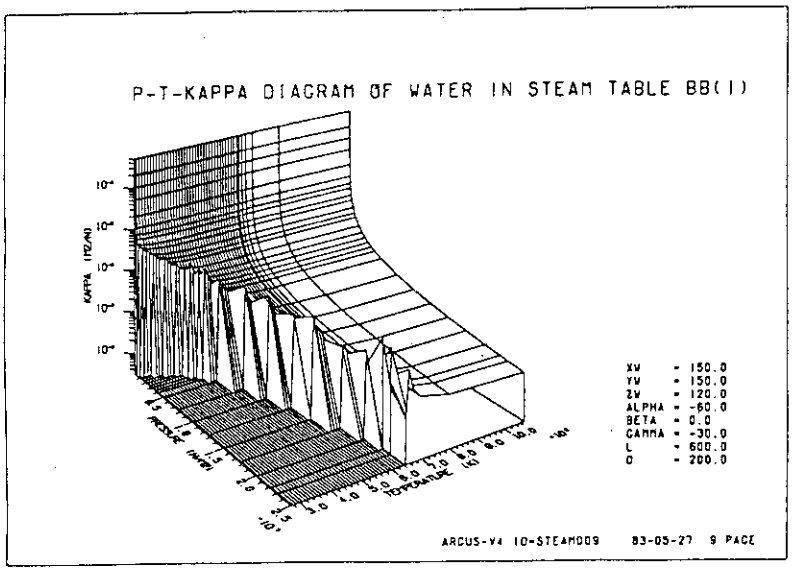


Fig. 5-3 P-T-β Diagram of Steam Tables





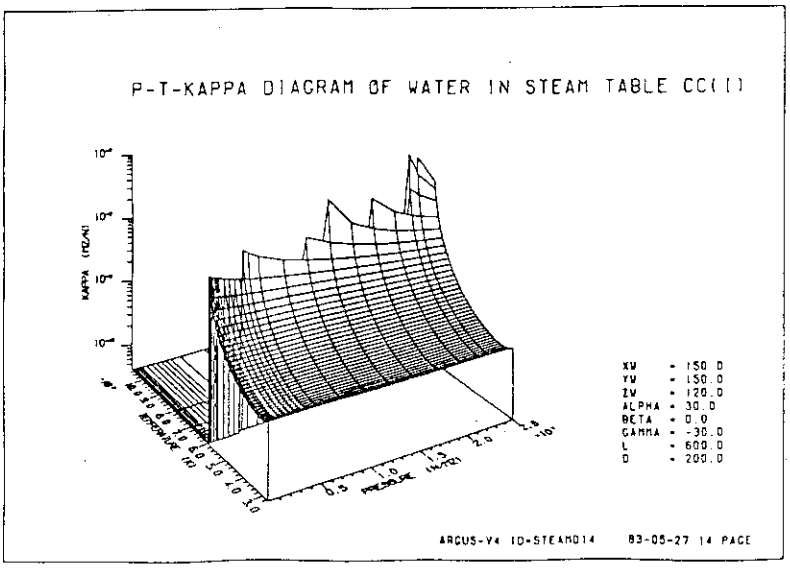
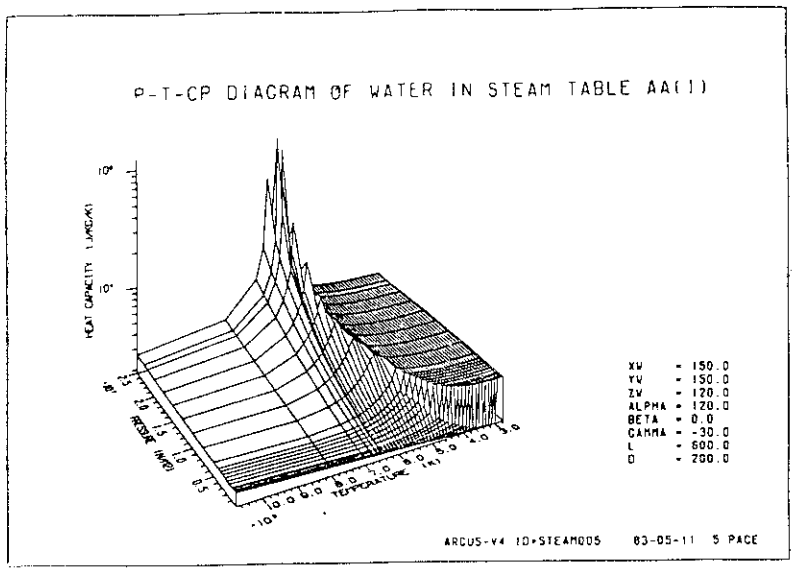
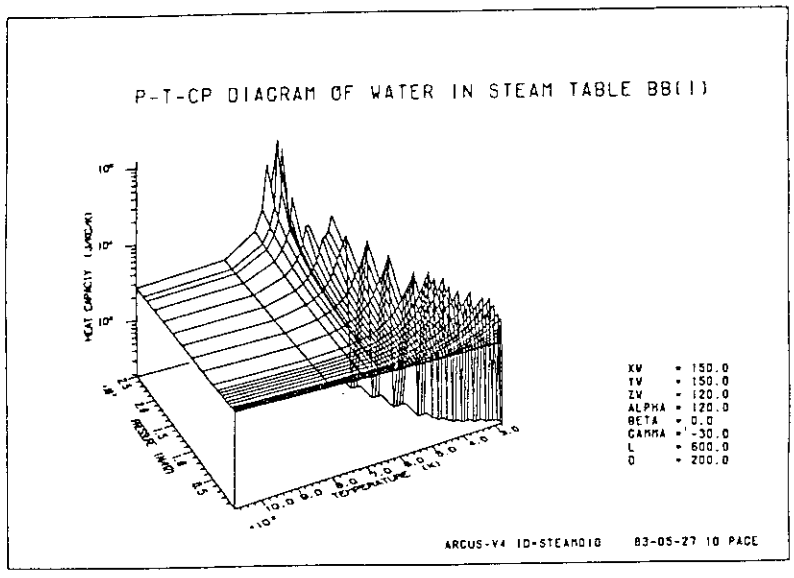


Fig. 5-4 P-T-κ Diagram of Steam Tables





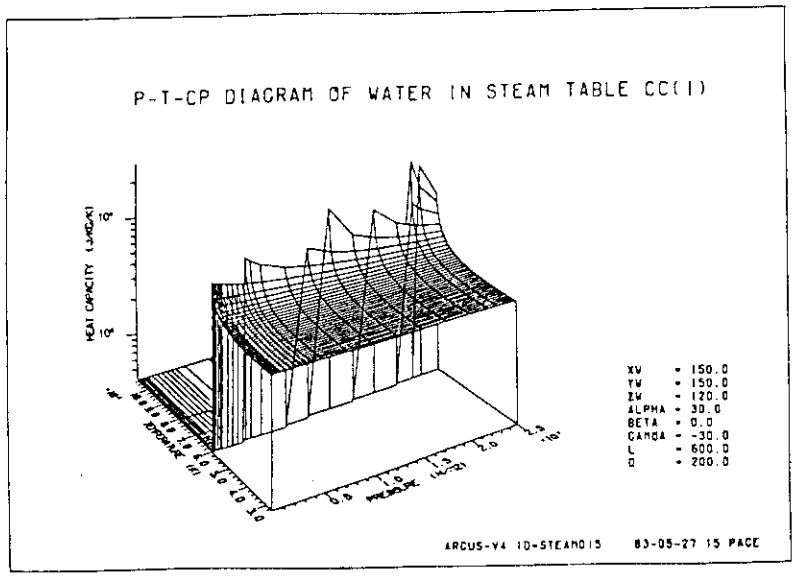
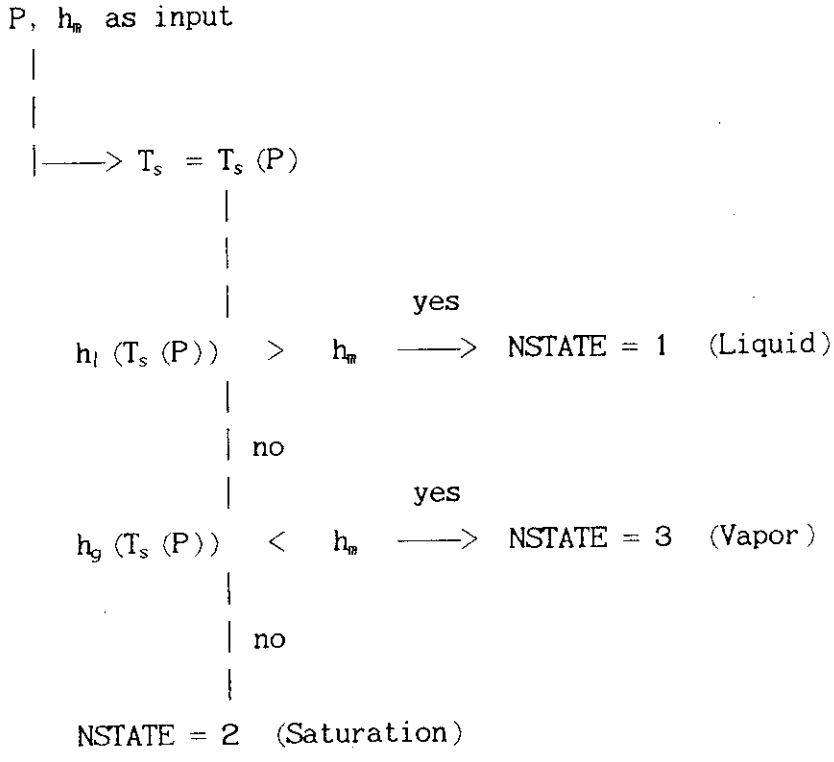


Fig. 5-5 P-T-C_p Diagram of Steam Tables

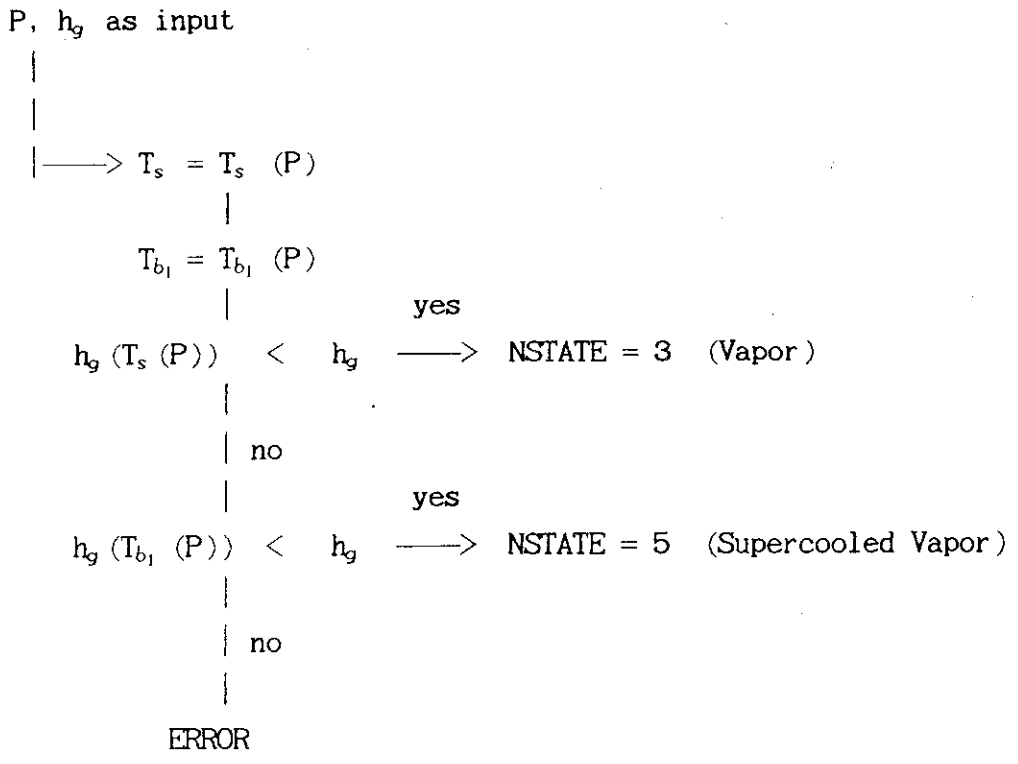
3. EXPANSION OF THE STH205 SUBROUTINE FOR THE METASTABLE STATES

The original subroutine "STH205"[7] uses the table to calculate the thermodynamic properties in the stable states and at the saturation state. The new subroutines "STH05G" and "STH05L" use the tables to compute the properties of vapor and liquid, respectively, in the stable and metastable states. Each subroutine has been made by improving the subroutine "STH205". "STH05G" or "STH05L" contains the interpolation routines corresponding only to the vapor or liquid state, respectively. The processes of interpolation of the tabular data and the thermodynamic relations are assumed to be equivalent in both metastable and stable states for each phase. The subroutines calculate the properties such as specific volume, specific internal energy, specific enthalpy, β, κ and C_p. using input data of pressure and enthalpy. Major flow charts for these subroutines are shown as follows.

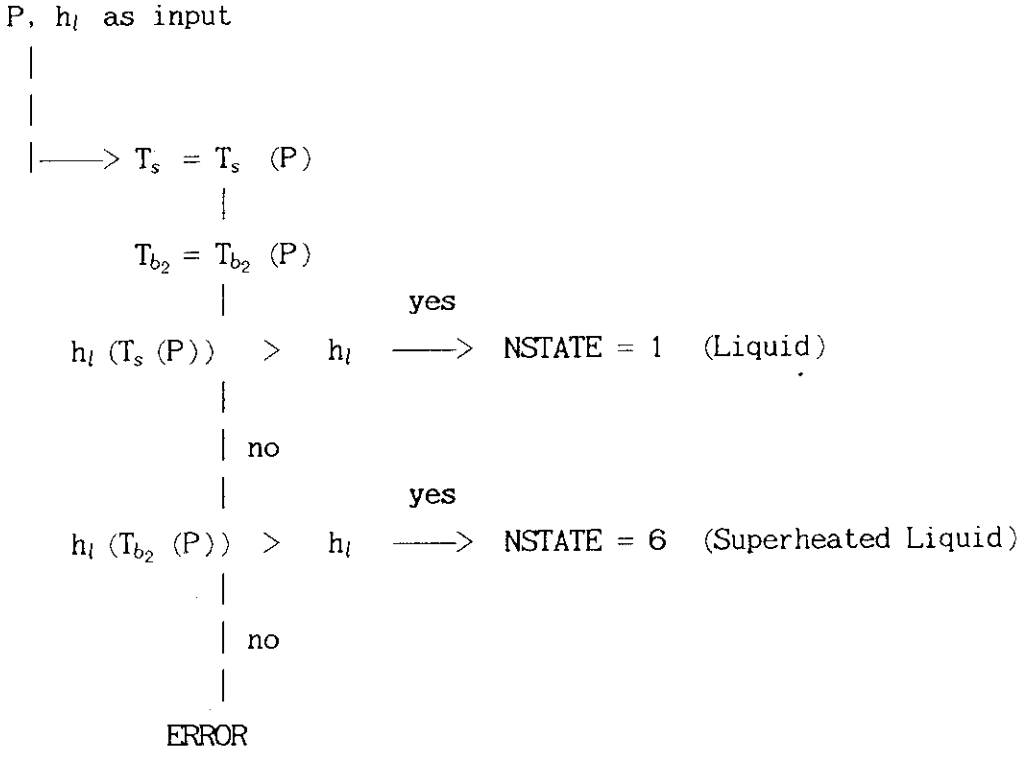
MAJOR FLOW SCHEME OF "STH205"



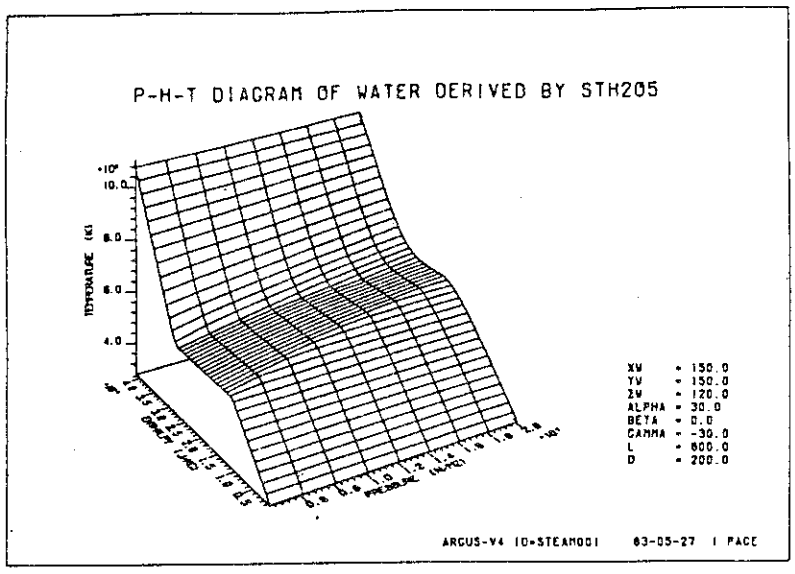
MAJOR FLOW SCHEME OF "STHO5G"

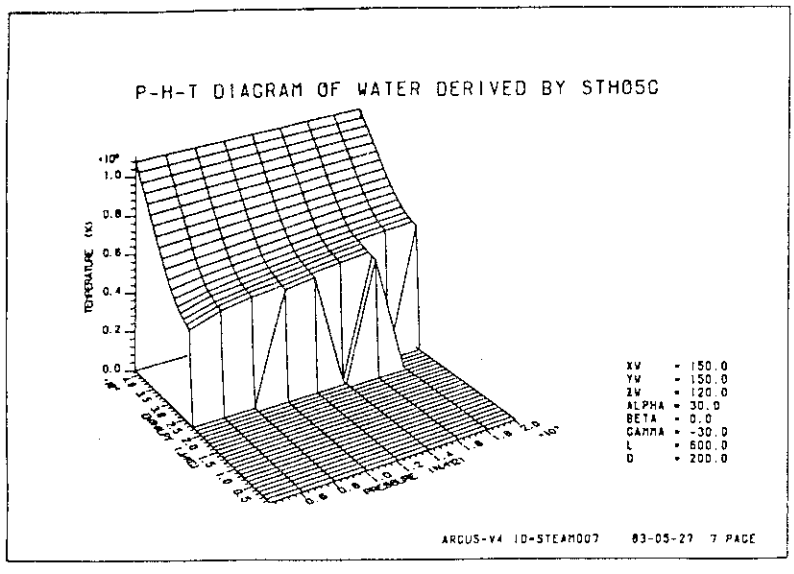


MAJOR FLOW SCHEME OF "STHO5L"



Figures 6-1 through 6-6 show the physical properties of water at input data of pressure and enthalpy which are calculated by these subroutines. The figures show that the IFC formulation can be extended smoothly into the metastable liquid. As for the metastable vapor, the formulation behaves well for the properties of specific volume and specific internal energy. It is not so good, however, for C_p, β and κ specially in the region of pressure above 1.4×10^7 N/m^2. The IFC formulation can not be well extrapolated in this region of vapor.





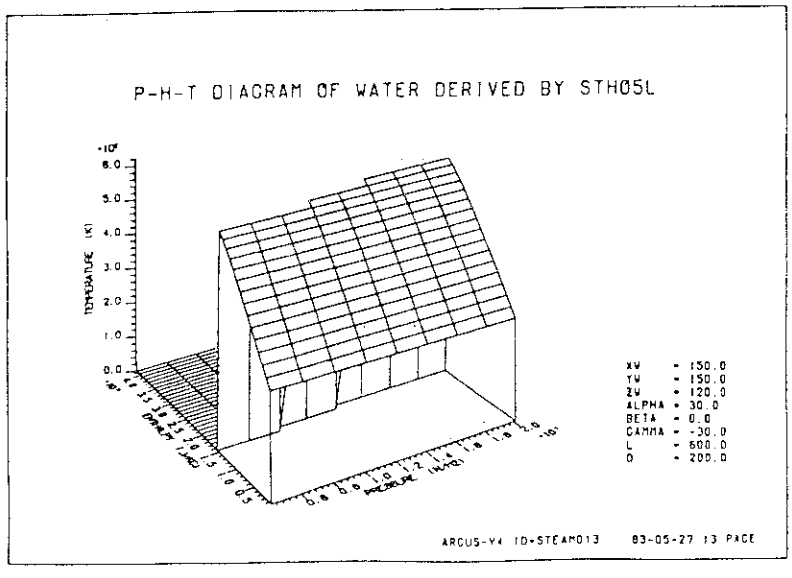
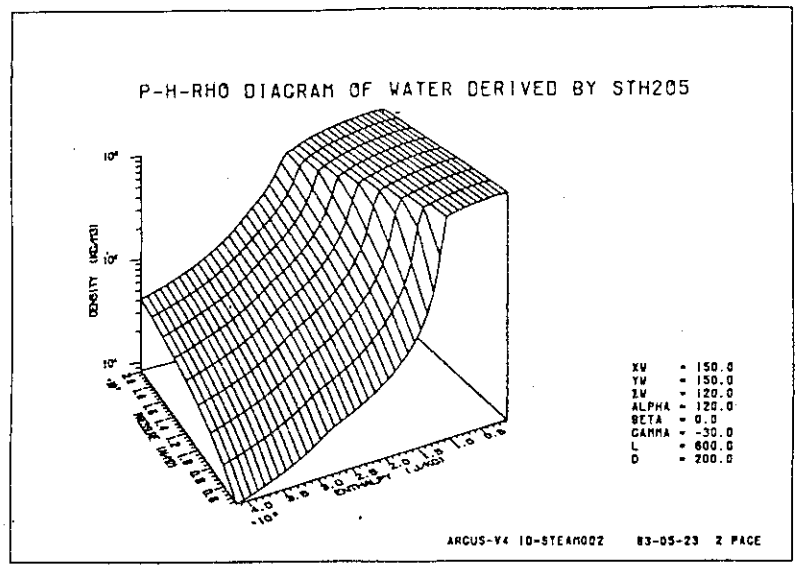
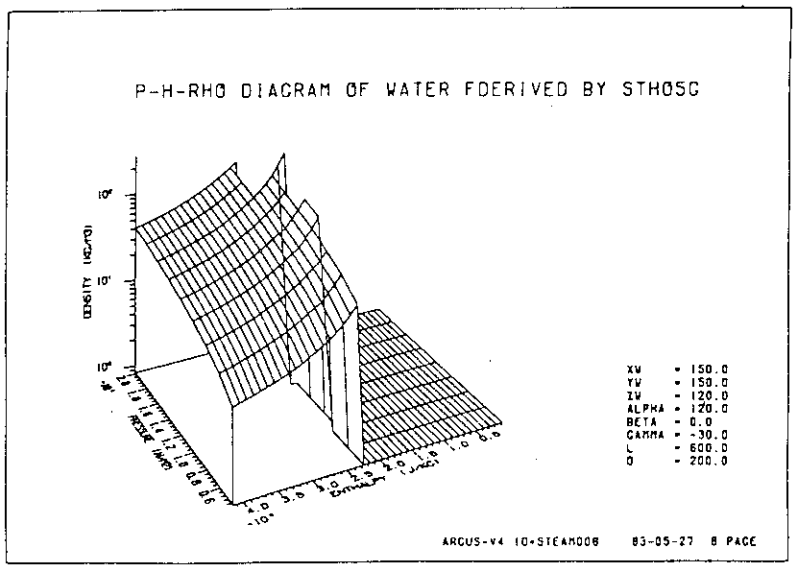


Fig. 6-1 P-h-T Diagram of Steam Tables





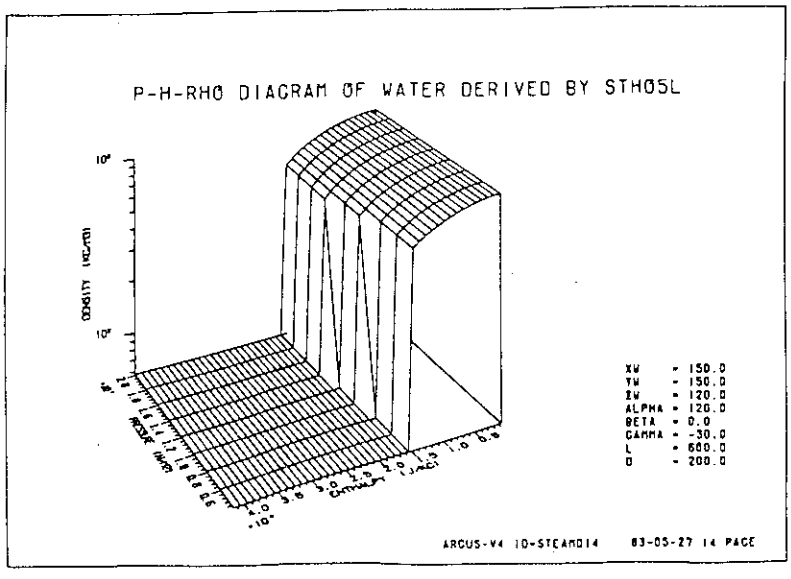
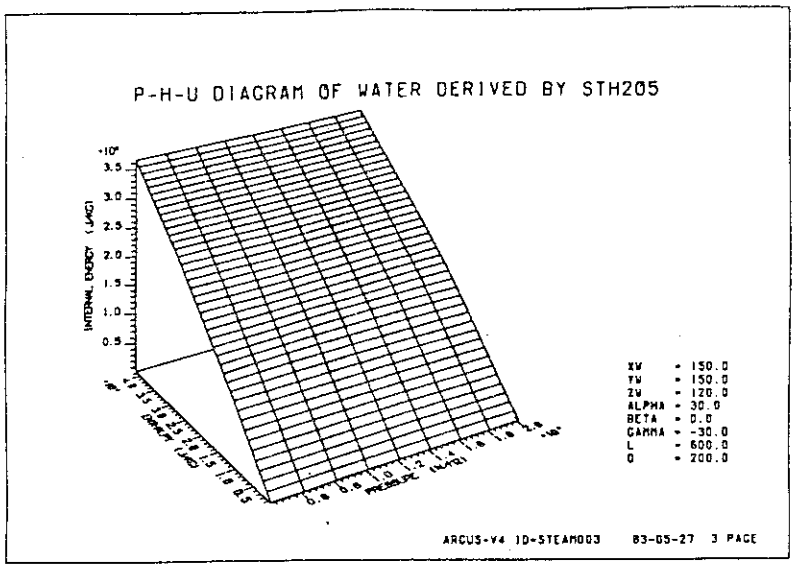
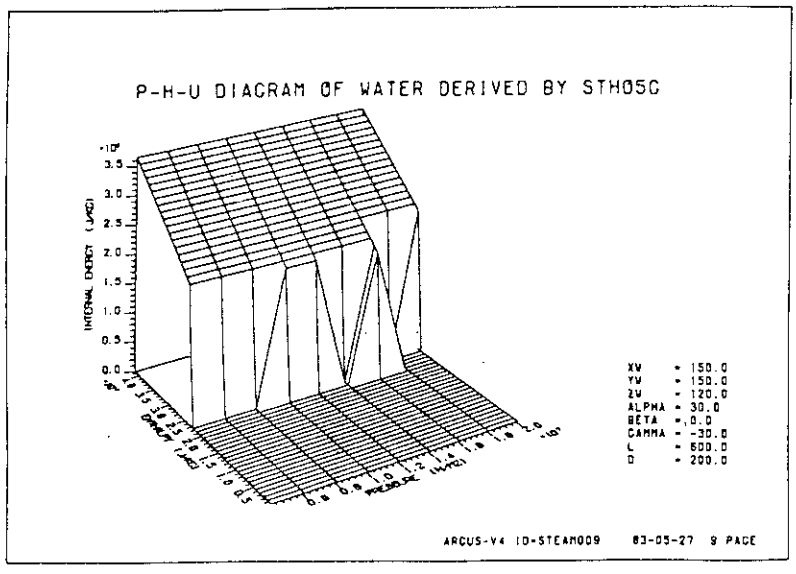


Fig. 6-2 P-h-1/v Diagram of Steam Tables





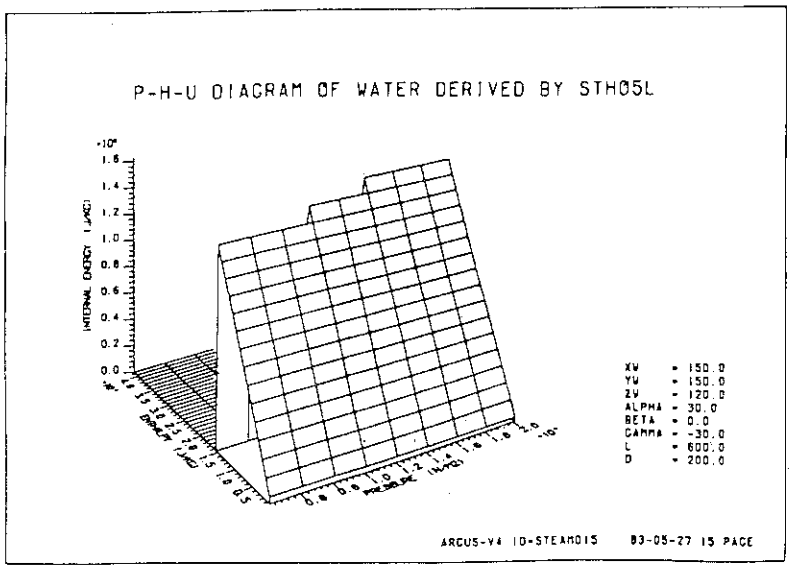
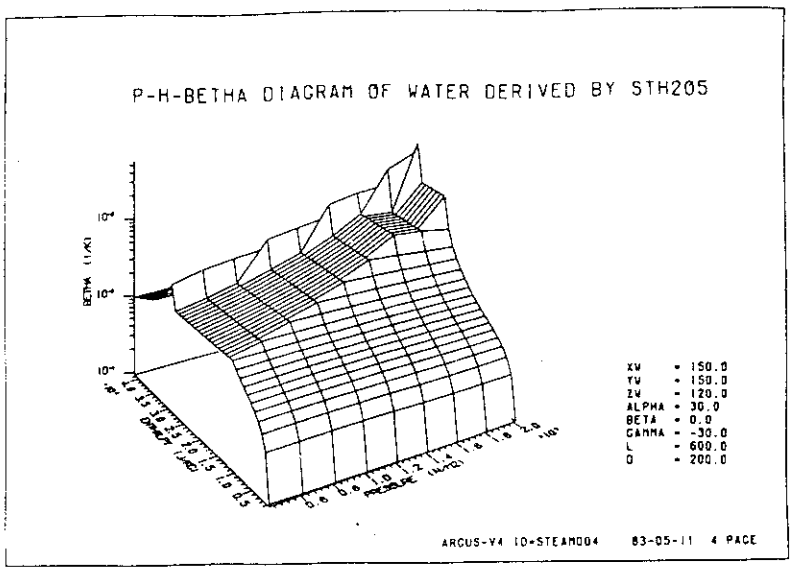
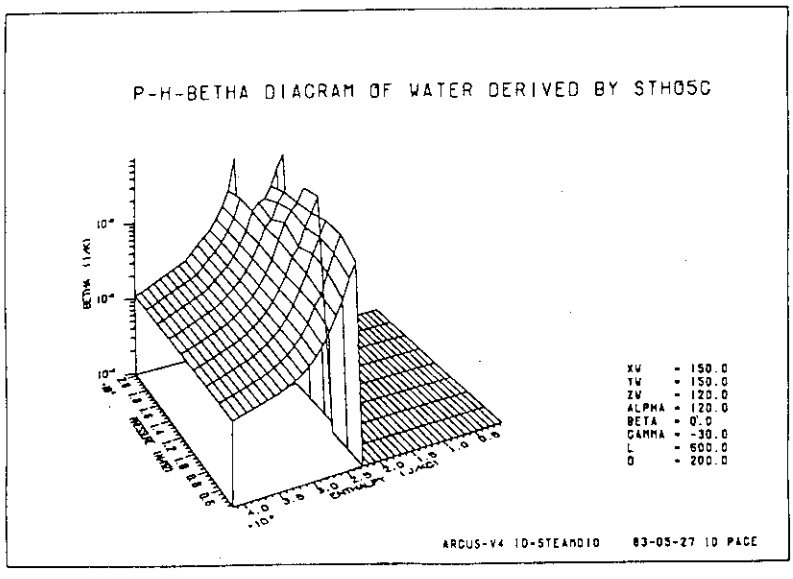


Fig. 6-3 P-h-u Diagram of Steam Tables





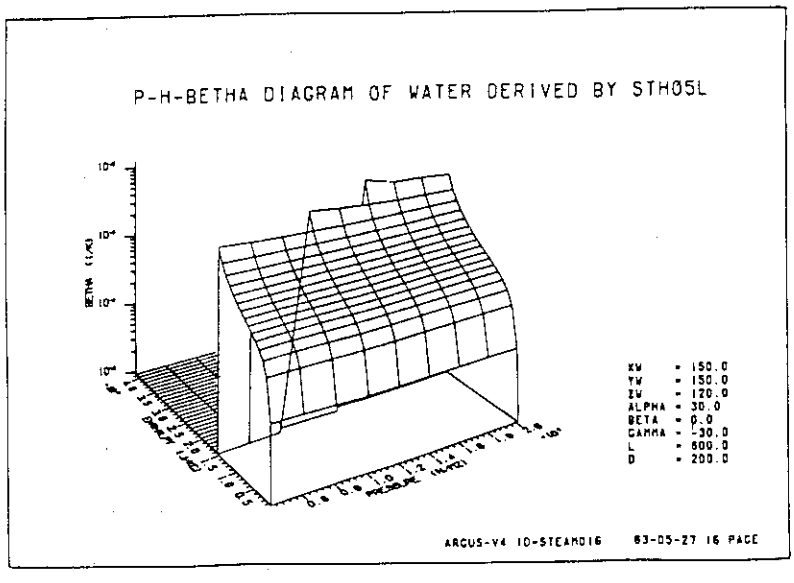
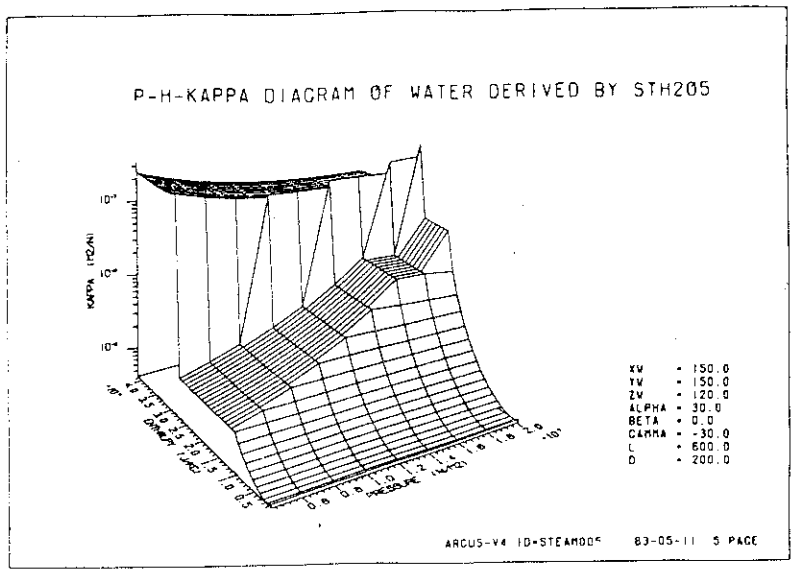
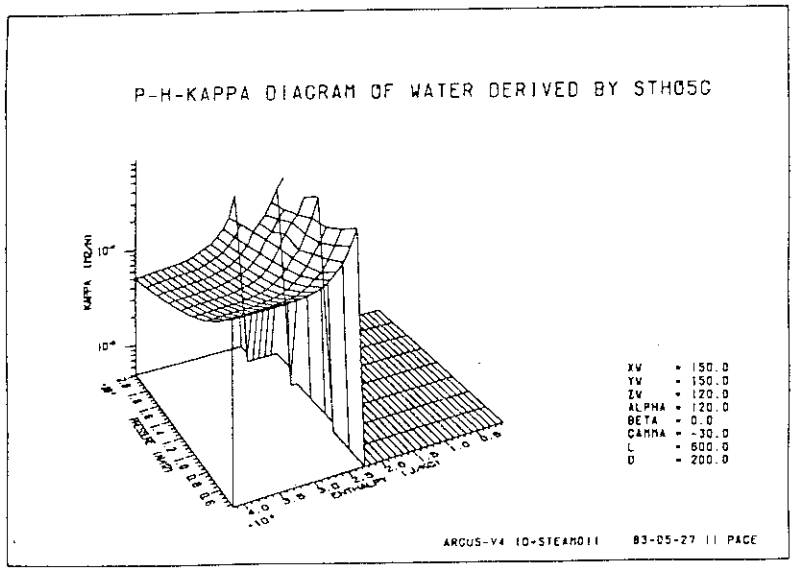


Fig. 6-4 P-h-β Diagram of Steam Tables





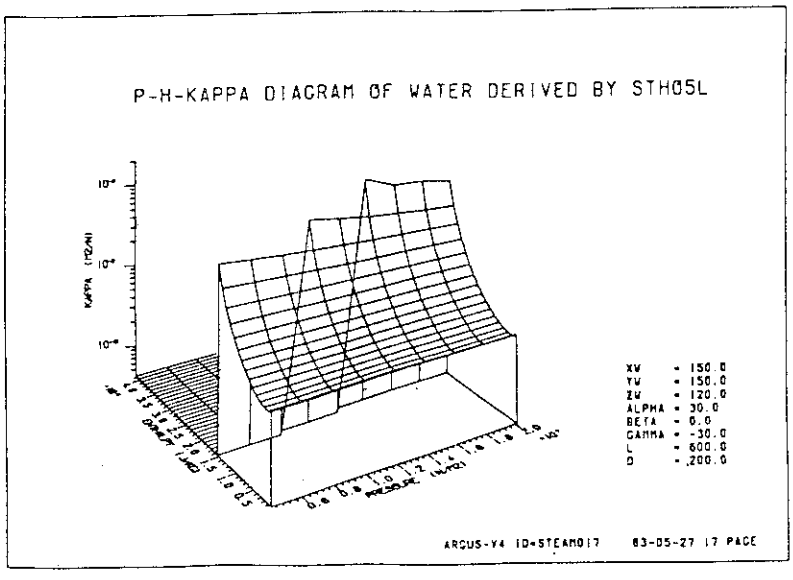
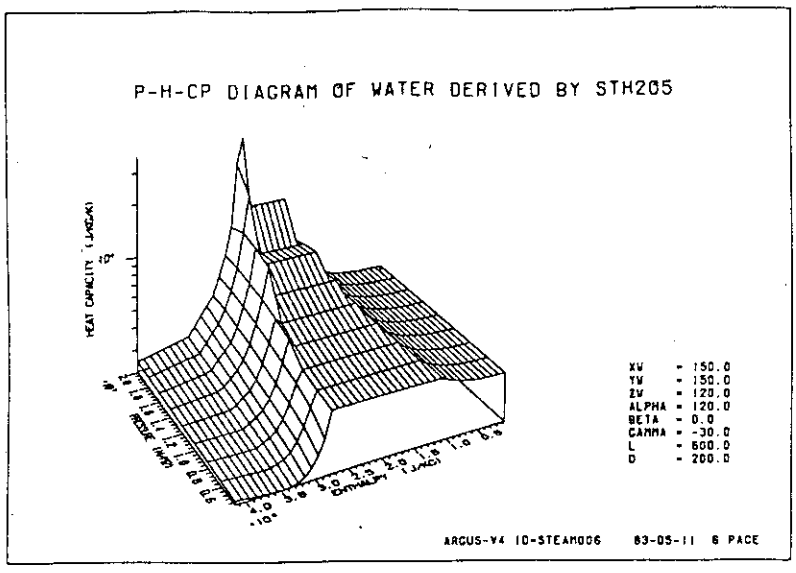
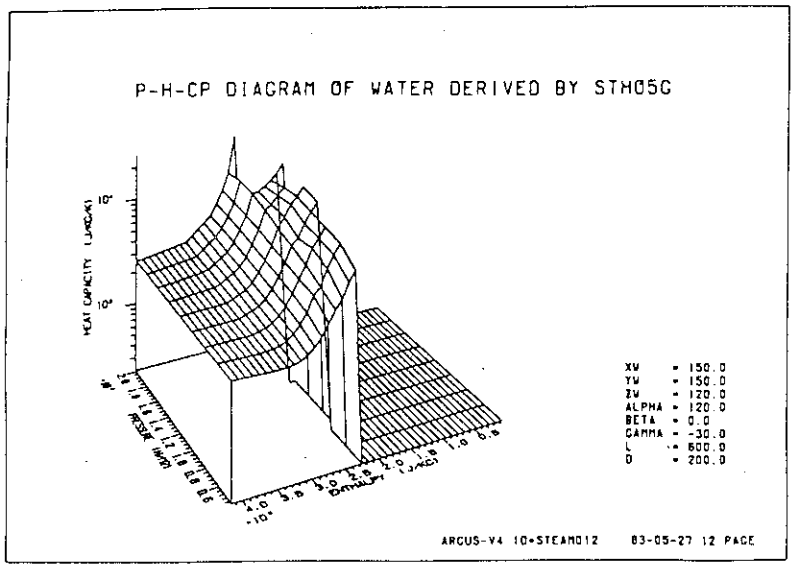


Fig. 6-5 P-h-κ Diagram of Steam Tables





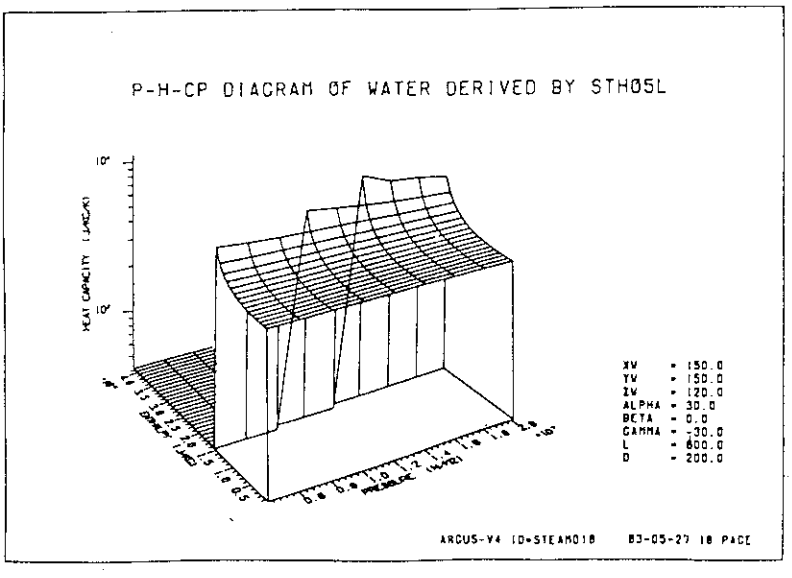


Fig. 6-6 P-h-C_p Diagram of Steam Tables

4. USAGE OF THE STH20 PROGRAM INCLUDING STH05G and STH05L

The "STH20" program[7] has several subroutines that use the tables to calculate water properties. The subroutine, "STH205", "STH05G" or "STH05L" is called as follow:

CALL STH205, STH05G or STH05L (NSTATE, S)

NSTATE :States ID (Return Value)
- =1 Subcooled Liquid
- =2 Saturated
- =3 Superheated Vapor
- =4 Supercritical
- =5 Supercooled Vapor
- =6 Superheated Liquid

S :Steam Table's Argument Values

	For STH05G	For STH05L	For STH205
S(1)	T_g	T_l	T
S(2)	P	P	P
S(3)	v_g	v_l	v
S(4)	u_g	u_l	u
S(5)	h_g	h_l	h
S(6)	β_g	β_l	β
S(7)	κ_g	κ_l	κ
S(8)	C_{pg}	C_{pl}	C_p
S(9)			x

S(10)	T_s or T_{b_1}	T_s or T_{b_2}	T_s
S(11)			v_{ls}
S(12)			v_{gs}
S(13)			u_{ls}
S(14)			u_{gs}
S(15)			h_{ls}
S(16)			h_{gs}
S(17)			β_{ls}
S(18)			β_{gs}
S(19)			κ_{ls}
S(20)			κ_{gs}
S(21)			C_{pls}
S(22)			C_{pgs}
S(23)	Indexes	Indexes	Indexes

In 'STH05G' and 'STH05L', S(9) and S(11) through S(22) are not defined. The indexes in S(23) are used to start the table search.

The subroutine 'STH20I' retrieves the table needed by the subroutines 'STH205', 'STH05G' and 'STH05L' and is called by the following fortran statement.

CALL STH20I (AA, BB, CC, N, NUSE, NUSE1)

AA, BB, CC :Steam Table Data Array

N :Steam Table Data I/O Reference Number

NUSE, NUSE1 : Array Size

On entry, NUSE and NUSE1 must be greater than or set equal to the length of the generated table(NTOT). On return, NUSE and NUSE1 are the number of words used in the arrays(NSIZE and NSIZE1).

5. CONCLUDING REMARKS

It has been presented as an application to reactor safety analysis that the physical properties of water in the metastable states are given by extrapolations of the IFC equations of state into the metastable regions. The obtained steam tables contains the wide range of thermodynamic states of water: subcooled, superheated, saturated liquid and vapor. Our steam tables can be used in unequal temperature models for transient two-phase flow. The extension of the subroutine "STH205" gives the relatively short time of computation to determine the thermodynamic properties at input data of pressure and enthalpy using the tabular data. Only the subroutine "STH205" has been improved, but it is possible to further improve the other subroutines which compute the thermodynamic quantities using other given properties as input. It has been shown that the IFC formulation behaves badly near the critical point in the metastable states. The data of β, κ and C_p are not extended smoothly into the metastable vapor in the region of above pressure 1.4×10^7 N/m^2. It is necessary that the formulation will be improved in this region. The values of the properties in the metastable states should be tested by the experimental results (for example, experimental flashing data).

N :Steam Table Data I/O Reference Number

NUSE, NUSE1 : Array Size

On entry, NUSE and NUSE1 must be greater than or set equal to the length of the generated table(NTOT). On return, NUSE and NUSE1 are the number of words used in the arrays(NSIZE and NSIZE1).

5. CONCLUDING REMARKS

It has been presented as an application to reactor safety analysis that the physical properties of water in the metastable states are given by extrapolations of the IFC equations of state into the metastable regions. The obtained steam tables contains the wide range of thermodynamic states of water: subcooled, superheated, saturated liquid and vapor. Our steam tables can be used in unequal temperature models for transient two-phase flow. The extension of the subroutine "STH2O5" gives the relatively short time of computation to determine the thermodynamic properties at input data of pressure and enthalpy using the tabular data. Only the subroutine "STH2O5" has been improved, but it is possible to further improve the other subroutines which compute the thermodynamic quantities using other given properties as input. It has been shown that the IFC formulation behaves badly near the critical point in the metastable states. The data of β, κ and C_p are not extended smoothly into the metastable vapor in the region of above pressure 1.4×10^7 N/m^2. It is necessary that the formulation will be improved in this region. The values of the properties in the metastable states should be tested by the experimental results (for example, experimental flashing data).

Nomenclatures

The nomenclatures used in this paper and the units of the properties are:

T	Temperature	K
P	Pressure	N/m^2
v	Specific Volume	m^3/kg
u	Specific Internal Energy	J/kg
h	Enthalpy	J/kg
β	Coefficient of thermal expansion	1/K
κ	Isothermal compressibility	m^2/N
C_p	Heat Capacity at Constant Pressure	J/(kg K)
x	Quality	
l	Liquid Subscript	
g	Vapor Subscript	
s	Saturated Quantity Subscript	
m	Mixture Subscript	
c	Critical Quantity Subscript	
r	Reduced Quantity Subscript	
b_{1or2}	Metastability Limit Subscript	
sp	Spinodal Line Subscript	
M	Maximum Superheat Subscript	

Acknowledgements

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REFERENCES

1) ASME Steam Table, "Thermodynamic and Transport Properties of Steam", 3rd Edition prepared by the ASME Committee on Properties of Steam, (1977).

2) O. C. Jones, Jr and P. Saha, *Non-Equilibrium Aspects of Water Reactor Safety*, "Thermal and Hydraulic Aspects of Nuclear Reactor Safety" in the Symposium on the Thermal and Hydraulic Aspects of Nuclear Reactor Safety, pp249-288, Vol.1, (1977).

3) F. Bakhtar and M. Piran, *Thermodynamic Properties of Supercooled Steam*, International Journal of Heat and Fluid, pp53-62, Vol. 1, (1979).

4) A. Karimi and J. H. Lienhard, *Toward a Fundamental Equation for Water in the Metastable States*, High Temperatures- High Pressures, pp511-517, Vol. 11, (1979).

5) RELAP5/MOD1, NUREG/CR-1826, (1980).

6) TRAC-PD2, *An Advanced Best-Estimate Computer Program for Pressurized Water Reactor Loss-of-Coolant Accident Analysis*, NUREG/CR-2054, (1981).

7) RELAP4/MOD5, *A Computer Program for Transient Thermal-Hydraulic Analysis of Nuclear Reactors and Related Systems*, ANCR-NUREG-1335, (1976).

8) K. Kobayashi, K. Nakatame, M. Akimoto, M. Okazaki, S. Sasaki, K. Soda and K. Sanokawa, *Digital Computer Subroutine STEAM for JSME STEAM TABLE*, JAERI-M-6967, (1977).

9) S. Inoue, T. Fujimura, T. Tsutsui and T. Nishida, *Mannual for JSSL* (JAERI Scientific Subroutine Library), JAERI-M-82-095, (1982).

10) G. V. Ermakov and V. P. Skripov, *Equation of State and Stability Boundary of a Metastable Liquid*, Teplofizika Vysokikh Temperatur, pp976-982, Vol.5, (1970).

11) V. P. Skripov and P. A. Pavlov, *Explosive Boiling of Liquids and Fluctuation Nucleus Formation*, Teplofizika Vysokikh Temperatur,

pp833-839, Vol.8, (1970).

12) P. A. Pavlov and V. P. Skripov, *Kinetics of Spontaneous Nucleation in Strongly Heated Liquids*, Teplofizika Vysokikh Temperatur, pp579-585, Vol. 8, (1970).

13) J. H. Lienhard, *Correlation for the Limiting Liquid Superheat*, Chemical Engineering Science, pp847-849, Vol. 31, (1976).

14) J. H. Lienhard and A. H. Karimi, *Corresponding States Correlations of the Extreme Liquid Superheat and Vapor Subcooling*, Transactions of the ASME, pp492-495, Vol. 100, (1978).

15) J. H. Lienhard and V. E. Schrock, *Generalized Displacement of the Nucleate Boiling Heat-Flux Curve, with Pressure Change*, International Journal of Heat Mass Transfer, pp355-363, Vol. 9, (1966).

16) P. P. Wegener and A. A. Pouring, *Experiments on Condensation of Water Vapor by Homogeneous Nucleation in Nozzles*, The Physics of Fluids, pp352-361, Vol. 7, (1964).

17) H. L. Jaeger, E. L. Willson, P. G. Hill and K. C. Russell , *Nucleation of Supersaturated Vapors in Nozzles, I. H20 and NH3*, Journal of Chemical Physics, pp5380-5388, Vol. 51, (1969).

18) G. S. Springer, *Homogeneous Nucleation*, in Advance in Heat Transfer edited by T. F. Irvine, Jr. and J. P. Hartnett, pp281-346, Vol. 14, (1978).

19) D. Barschdorff, *Carrier Gas Effects on Homogeneous Nucleation of Water Vapor in a Shock Tube*, The Physics of Fluids, pp529-539, Vol. 18, (1975).

20) R. H. Heist and H. Reiss, *Investigation of the Homogeneous Nucleation of Water Vapor Using a Diffusion Cloud Chamber*, Journal of Chemical Physics, pp665-671, Vol. 59, (1973).

Appendix 1 Flow Scheme of Subroutine "STEAM" for Three Steam Tables

FLOW SCHEME OF "STEAM" FOR STEAM TABLE AA(I)

P, T as input ($T = T_m$)

|

|

|——> Subroutine "STEAM"

|

|

|——> NSTWAT=2 —— Physical Quantities of Liquid State
| at P_s (T) or T_s (P)
| v_l , u_l , β_l , κ_l , C_{pl}

|

|

|——> NSTWAT=1 —— Physical Quantities of Vapor State
| at P_s (T) and T_s (P)
| v_g , u_g , β_g , κ_g , C_{pg}

|

|

|——> NSTWAT=0 —— Physical Quantities in Subcooled Liquid
and Superheated Vapor State
v_l , u_l , β_l , κ_l , C_{pl} and
v_g , u_g , β_g , κ_g , C_{pg}

FLOW SCHEME OF "STEAM" FOR STEAM TABLE BB(I)

P, T as input ($T = T_g$)

|

|

|——> SUBROUTINE "STEAM"

|

|

|——> NSTWAT=1 —— Physical Quantities of Vapor State
| at P_s (T) and T_s (P)
| v_g , u_g , β_g , κ_g , C_{pg}

|

```
|
|---> NSTWAT=0 --- Physical Quantities of Vapor State
|                  at P_b1 (T) and T_b1 (P)
|                  v_g , u_g , β_g , κ_g , C_pg
|
|
|---> NSTWAT=0 --- Physical Quantities in Supercooled Vapor
                   and Superheated Vapor State
                   v_g , u_g , β_g , κ_g , C_pg  and
                   v_g'' , u_g'' , β_g'' , κ_g'' , C_pg''
```

FLOW SCHEME OF "STEAM" FOR STEAM TABLE CC(I)

```
P, T as input ( T = T_l )
 |
 |
 |-------> Subroutine "STEAM"
           |
           |
           |---> NSTWAT=2 --- Physical Quantities of Liquid State
           |                  at P_s (T) and T_s (P)
           |                  v_l , u_l , β_l , κ_l , C_pl
           |
           |
           |---> NSTWAT=0 --- Physical Quantities of Liquid State
           |                  at P_b2 (T) and T_b2 (P)
           |                  v_l , u_l , β_l , κ_l , C_pl
           |
           |
           |---> NSTWAT=0 --- Physical Quantities in Subcooled Liquid
                              and Superheated Liquid State
                              v_l , u_l , β_l , κ_l , C_pl  and
                              v_l' , u_l' , β_l' , κ_l' , C_pl'
```

Appendix 2 Equations of the Metastability Limits Obtained by the Extrapolations

(note: The units for temperature and pressure are here Celsius and $kg.f/cm^2$, which are used in the subroutine "STEAM".)

For the boundary of supercooled vapor

$0.00 < T < 100.0$ °C

$$P_{b_l}(T) = 0.16\,T + 4.0 \quad kg.f/cm^2$$

$100.0 < T < 180.0$

$$P_{b_l}(T) = 0.3125\,T - 11.25$$

$180.0 < T < 245.0$

$$P_{b_l}(T) = 0.6135\,T - 65.7485$$

$245.0 < T < 290.0$

$$P_{b_l}(T) = 0.8889\,T - 132.781$$

$290.0 < T < 310.0$

$$P_{b_l}(T) = 2.0\,T - 455.0$$

$310.0 < T < 354.0$

$$P_{b_l}(T) = 175.0$$

$354.0 < T < 374.15$

$$P_{b_l}(T) = \text{saturation line}$$

For the boundary of superheated liquid

$0.00 < T < 320.0$ °C

$P_{b_2}(T) = 0.0$ kg.f/cm^2

$320.0 < T < 345.0$

$P_{b_2}(T) = 4.7999872\ T - 1535.995584$

$345.0 < T < 360.0$

$P_{b_2}(T) = 10/3\ T - 1030.0$

$360.0 < T < 374.15$

$P_{b_2}(T)$ = saturation line

Appendix 3 Arrays of Steam Tables

ARRAY OF STEAM TABLE AA(I) (I=1, NSIZE)

NT = the number of temperatures entered as defined

NP = the number of pressures entered as defined

NS = the number of input temperature not above the critical temperature.

NS2= the number of input pressures not above the critical pressure.

NSIZE = NT + NP + 11 x NS + 11 x NS2 + 5 x NT x NP

. I = 1, ... , NT

AA(I) = T ($T = T_m$)

. I = NT + 1, ... , NT + NP

AA(I) = P

. I = NT + NP + 1, ... ,NT + NP + 11 x NS

AA(JPL + 11 x (K − 1) + 1) = B(1, K) = P_s (T)

AA(JPL + 11 x (K − 1) + 2) = B(2, K) = v_l (P_s(T))

AA(JPL + 11 x (K − 1) + 3) = B(3, K) = u_l (P_s(T))

AA(JPL + 11 x (K − 1) + 4) = B(4, K) = β_l (P_s(T))

AA(JPL + 11 x (K − 1) + 5) = B(5, K) = κ_l (P_s(T))

AA(JPL + 11 x (K − 1) + 6) = B(6, K) = C_{pl} (P_s(T))

AA(JPL + 11 x (K − 1) + 7) = B(7, K) = v_g (P_s(T))

$AA(JPL + 11 \times (K - 1) + 8) = B(8, K) = u_g \ (P_s(T))$

$AA(JPL + 11 \times (K - 1) + 9) = B(9, K) = \beta_g \ (P_s(T))$

$AA(JPL + 11 \times (K - 1) + 10) = B(10, K) = \kappa_g \ (P_s(T))$

$AA(JPL + 11 \times (K - 1) + 11) = B(11, K) = C_{pg}(P_s(T))$

where $JPL = NT + NP$ and $K = 1, \ldots\ldots, NS$.

. $I = JPL + 11 \times NS + 1, \ldots\ldots, JPL + 11 \times NS + 11 \times NS2$

$AA(JP1 + 11 \times (L - 1) + 1) = C(1, L) = T_s \ (P)$

$AA(JP1 + 11 \times (L - 1) + 2) = C(2, L) = v_l \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 3) = C(3, L) = u_l \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 4) = C(4, L) = \beta_l \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 5) = C(5, L) = \kappa_l \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 6) = C(6, L) = C_{pl}(T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 7) = C(7, L) = v_g \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 8) = C(8, L) = u_g \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 9) = C(9, L) = \beta_g \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 10) = C(10, L) = \kappa_g \ (T_s(P))$

$AA(JP1 + 11 \times (L - 1) + 11) = C(11, L) = C_{pg}(T_s(P))$

where $JP1 = NT + NP + 11 \times NS$ and $L = 1, \ldots\ldots, NS2$.

. $I = JP1 + 11 \times NS2 + 1, \ldots\ldots, JP1 + 11 \times NS2 + 5 \times NT \times NP$

$$AA(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 1) = D\ (1, N, J)$$
$$= v_l\ (P, T) \text{ or } v_g\ (P, T)$$
$$AA(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 2) = D\ (2, N, J)$$
$$= u_l\ (P, T) \text{ or } u_g\ (P, T)$$
$$AA(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 3) = D\ (3, N, J)$$
$$= \beta_l\ (P, T) \text{ or } \beta_g\ (P, T)$$
$$AA(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 4) = D\ (4, N, J)$$
$$= \kappa_l\ (P, T) \text{ or } \kappa_g\ (P, T)$$
$$AA(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 5) = D\ (5, N, J)$$
$$= C_{pl}\ (P, T) \text{ or } C_{pg}\ (P, T)$$

where $N = 1, \ldots\ldots, NT$, $J = 1, \ldots\ldots, NP$ and $JP2 = JP1 + 11 \times NS2$.

ARRAY OF STEAM TABLE BB(I) (I=1, NSIZE1)

NSIZE1 =NT + NP + 12 x NS + 12 x NS2 + 5 x NT x NP

. I = 1,....., NT

BB(I) = T ($T = T_g$)

. I = NT + 1,....., NT + NP

BB(I) = P

. I = NT + NP + 1,.....,NT + NP + 12 x NS

BB(JPL + 12 x (K − 1) + 1) = B(1, K) = P_s (T)

BB(JPL + 12 x (K − 1) + 2) = B(2, K) = v_g (P_{b_l}(T))

BB(JPL + 12 x (K − 1) + 3) = B(3, K) = u_g (P_{b_l}(T))

BB(JPL + 12 x (K − 1) + 4) = B(4, K) = β_g (P_{b_l}(T))

BB(JPL + 12 x (K − 1) + 5) = B(5, K) = κ_g (P_{b_l}(T))

BB(JPL + 12 x (K − 1) + 6) = B(6, K) = C_{pg}(P_{b_l}(T))

BB(JPL + 12 x (K − 1) + 7) = B(7, K) = v_g (P_s(T))

BB(JPL + 12 x (K − 1) + 8) = B(8, K) = u_g (P_s(T))

BB(JPL + 12 x (K − 1) + 9) = B(9, K) = β_g (P_s(T))

BB(JPL + 12 x (K − 1) + 10) = B(10, K) = κ_g (P_s(T))

BB(JPL + 12 x (K − 1) + 11) = B(11, K) = C_{pg}(P_s(T))

BB(JPL + 12 x (K − 1) + 12) = B(12, K) = P_{b_l}(T)

where JPL = NT + NP and K = 1, ... , NS.

. I = JPL + 12 x NS + 1, ... , JPL + 12 x NS + 12 x NS2

$BB(JP1 + 12 \times (L - 1) + 1) = C(1, L) = T_s\ (P)$

$BB(JP1 + 12 \times (L - 1) + 2) = C(2, L) = v_g\ (T_{b_l}(P))$

$BB(JP1 + 12 \times (L - 1) + 3) = C(3, L) = u_g\ (T_{b_l}(P))$

$BB(JP1 + 12 \times (L - 1) + 4) = C(4, L) = \beta_g\ (T_{b_l}(P))$

$BB(JP1 + 12 \times (L - 1) + 5) = C(5, L) = \kappa_g\ (T_{b_l}(P))$

$BB(JP1 + 12 \times (L - 1) + 6) = C(6, L) = C_{pg}(T_{b_l}(P))$

$BB(JP1 + 12 \times (L - 1) + 7) = C(7, L) = v_g\ (T_s(P))$

$BB(JP1 + 12 \times (L - 1) + 8) = C(8, L) = u_g\ (T_s(P))$

$BB(JP1 + 12 \times (L - 1) + 9) = C(9, L) = \beta_g\ (T_s(P))$

$BB(JP1 + 12 \times (L - 1) + 10) = C(10, L) = \kappa_g\ (T_s(P))$

$BB(JP1 + 12 \times (L - 1) + 11) = C(11, L) = C_{pg}(T_s(P))$

$BB(JP1 + 12 \times (L - 1) + 12) = C(12, L) = T_{b_l}(P)$

where JP1 = NT + NP + 12 x NS and L = 1, ... , NS2.

. I = JP1 + 12 x NS2 + 1, ... , JP1 + 12 x NS2 + 5 x NT x NP

$BB(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 1) = D\ (1, N, J) = v_g\ (P, T)$ or $v_g^m\ (P, T)$

$BB(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 2) = D\ (2, N, J) = u_g\ (P, T)$ or $u_g^m\ (P, T)$

$BB(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 3) = D\ (3, N, J) = \beta_g\ (P, T)$ or $\beta_g^m\ (P, T)$

$$BB(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 4) = D \quad (4, N, J)$$
$$= \kappa_g \quad (P, T) \text{ or } \kappa_g^* (P, T)$$
$$BB(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 5) = D \quad (5, N, J)$$
$$= C_{pg} \quad (P, T) \text{ or } C_{pg}^* (P, T)$$

where $N = 1, \ldots\ldots, NT$, $J = 1, \ldots\ldots, NP$ and $JP2 = JP1 + 12 \times NS2$.

ARRAY OF STEAM TABLE CC(I) (I=1, NSIZE1)

. I = 1, ... , NT

CC(I) = T ($T = T_l$)

. I = NT + 1, ... , NT + NP

CC(I) = P

. I = NT + NP + 1, ... ,NT + NP + 12 x NS

CC(JPL + 12 x (K − 1) + 1) = B(1, K) = P_s (T)

CC(JPL + 12 x (K − 1) + 2) = B(2, K) = v_l (P_s(T))

CC(JPL + 12 x (K − 1) + 3) = B(3, K) = u_l (P_s(T))

CC(JPL + 12 x (K − 1) + 4) = B(4, K) = β_l (P_s(T))

CC(JPL + 12 x (K − 1) + 5) = B(5, K) = κ_l (P_s(T))

CC(JPL + 12 x (K − 1) + 6) = B(6, K) = C_{pl} (P_s(T))

CC(JPL + 12 x (K − 1) + 7) = B(7, K) = v_l (P_{b_2}(T))

CC(JPL + 12 x (K − 1) + 8) = B(8, K) = u_l (P_{b_2}(T))

CC(JPL + 12 x (K − 1) + 9) = B(9, K) = β_l (P_{b_2}(T))

CC(JPL + 12 x (K − 1) + 10) = B(10, K) = κ_l (P_{b_2}(T))

CC(JPL + 12 x (K − 1) + 11) = B(11, K) = C_{pl} (P_{b_2}(T))

CC(JPL + 12 x (K − 1) + 12) = B(12, K) = P_{b_2}(T)

where JPL = NT + NP and K = 1, ... , NS.

. I = JPL + 12 x NS + 1, ... , JPL + 12 x NS + 12 x NS2

$CC(JP1 + 12 \times (L - 1) + 1) = C(1, L) = T_s\ (P)$

$CC(JP1 + 12 \times (L - 1) + 2) = C(2, L) = v_l\ (T_s(P))$

$CC(JP1 + 12 \times (L - 1) + 3) = C(3, L) = u_l\ (T_s(P))$

$CC(JP1 + 12 \times (L - 1) + 4) = C(4, L) = \beta_l\ (T_s(P))$

$CC(JP1 + 12 \times (L - 1) + 5) = C(5, L) = \kappa_l\ (T_s(P))$

$CC(JP1 + 12 \times (L - 1) + 6) = C(6, L) = C_{pl}(T_s(P))$

$CC(JP1 + 12 \times (L - 1) + 7) = C(7, L) = v_l\ (T_{b_2}(P))$

$CC(JP1 + 12 \times (L - 1) + 8) = C(8, L) = u_l\ (T_{b_2}(P))$

$CC(JP1 + 12 \times (L - 1) + 9) = C(9, L) = \beta_l\ (T_{b_2}(P))$

$CC(JP1 + 12 \times (L - 1) + 10) = C(10, L) = \kappa_l\ (T_{b_2}(P))$

$CC(JP1 + 12 \times (L - 1) + 11) = C(11, L) = C_{pl}(T_{b_2}(P))$

$CC(JP1 + 12 \times (L - 1) + 12) = C(12, L) = T_{b_2}(P)$

where JP1 = NT + NP + 12 x NS and L = 1, ... , NS2.

. I = JP1 + 12 x NS2 + 1, ... , JP1 + 12 x NS2 + 5 x NT x NP

$CC(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 1) = D\ (1, N, J)$
$= v_l\ (P, T)$ or $v_l'\ (P, T)$

$CC(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 2) = D\ (2, N, J)$
$= u_l\ (P, T)$ or $u_l'\ (P, T)$

$CC(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 3) = D\ (3, N, J)$
$= \beta_l\ (P, T)$ or $\beta_l'\ (P, T)$

$CC(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 4) = D\ (4, N, J)$
$= \kappa_l\ (P, T)$ or $\kappa_l'\ (p, T)$

$$CC(JP2 + 5 \times (N - 1) + 5 \times NT \times (J - 1) + 5) = D \quad (5, N, J)$$
$$= C_{pl} \ (P, T) \text{ or } C_{pl}' \ (P, T)$$

where N = 1,....., NT, J = 1,....., NP and JP2 = JP1 + 12 x NS2.

Appendix 4 Application of STHOSG and STHOSL to Separate Energy Model for Two Phase Flow

The field balance equations are used to obtain the state dependent variables changing with space and time in the flow field. These field equations do not constitute a closed equation system until an equation of state is specified together with the wall and interphase relationships. The numerical solution methods such as a non-linear implicit method also require that the thermodynamic properties be linearized about a known iteration level in order to solve for the dependent variables at the next iteration level. If the separate energy levels for each phase in the mixture is introduced into the field balance equation, the metastable states of the fluid should be allowed. Thermodynamic property data, in general, are not available for these states. As described in Section 2, thermodynamic properties for metastable states are assumed to be obtained in terms of the extrapolation of the IFC formulation within proper degree of metastable. Various thermodynamic relationships such as the Maxwell relations are also assumed to be satisfied in metastable states. In the present appendix, we outline the requirements of the equation of state for separate energy model (2T model) with general thermodynamic relations.

A.4.1 General Thermodynamic Relations

Supposing a thermodynamic variable Z which is a function of two other thermodynamic variables: X and Y, we have the following relationships:

$$\left(\frac{\partial X}{\partial Y}\right)_Z \left(\frac{\partial Y}{\partial Z}\right)_X \left(\frac{\partial Z}{\partial X}\right)_Y = -1 \quad , \tag{1}$$

$$\left(\frac{\partial M}{\partial Y}\right)_X = \left(\frac{\partial N}{\partial X}\right)_Y \quad , \tag{2}$$

where

$$M = \left(\frac{\partial Z}{\partial X}\right)_Y \quad , \qquad N = \left(\frac{\partial Z}{\partial Y}\right)_X \quad .$$

The first thermodynamic law gives

$$du = Tds - Pdv \quad (dq = Tds), \tag{3}$$

or $$dh = Tds + vdP \quad . \tag{4}$$

The specific heats at constant pressure and volume are defined by, respectively,

$$C_P = \left(\frac{\partial q}{\partial T}\right)_P = T\left(\frac{\partial S}{\partial T}\right)_P = \left(\frac{\partial h}{\partial T}\right)_P \quad , \tag{5}$$

$$C_v = \left(\frac{\partial q}{\partial T}\right)_v = T\left(\frac{\partial S}{\partial T}\right)_v = \left(\frac{\partial u}{\partial T}\right)_v \quad . \tag{6}$$

Helmholtz and Gibbs free energies are defined by, respectively,

$$f = U - Ts \quad , \tag{7}$$

$$g = h - Ts \quad . \tag{8}$$

Using the equations (3) and (4), we obtain the following expressions for the first thermodynamic law:

$$df = -sdT - Pdv \quad , \tag{9}$$

$$dg = -sdT + vdP \quad . \tag{10}$$

Using the equations (3), (4), (9) and (10), we obtain both exact differentials:

$$\left(\frac{\partial u}{\partial s}\right)_v = T = \left(\frac{\partial h}{\partial s}\right)_P \quad , \tag{11}$$

$$\left(\frac{\partial u}{\partial v}\right)_s = -P = \left(\frac{\partial f}{\partial v}\right)_T \quad , \tag{12}$$

$$\left(\frac{\partial h}{\partial P}\right)_s = v = \left(\frac{\partial g}{\partial P}\right)_T \quad , \tag{13}$$

$$\left(\frac{\partial f}{\partial T}\right)_v = -S = \left(\frac{\partial g}{\partial T}\right)_P \quad , \tag{14}$$

and the Maxwell relations:

$$\left(\frac{\partial T}{\partial v}\right)_s = -\left(\frac{\partial P}{\partial s}\right)_v \quad , \tag{15}$$

$$\left(\frac{\partial T}{\partial p}\right)_s = \left(\frac{\partial v}{\partial s}\right)_p \quad , \tag{16}$$

$$\left(\frac{\partial s}{\partial v}\right)_T = \left(\frac{\partial P}{\partial T}\right)_v \quad , \tag{17}$$

$$-\left(\frac{\partial s}{\partial p}\right)_T = \left(\frac{\partial v}{\partial T}\right)_p \quad . \tag{18}$$

Using equations (5), (6), (17) and (18), the dq (= Tds) can be expressed by the following:

$$\begin{aligned} dq &= \left(\frac{\partial q}{\partial T}\right)_P dT + \left(\frac{\partial q}{\partial P}\right)_T dP \quad , \\ &= C_p\, dT + T\left(\frac{\partial s}{\partial P}\right)_T dP \quad , \\ &= C_p\, dT - T\left(\frac{\partial v}{\partial T}\right)_p dP \quad , \end{aligned} \tag{19}$$

or

$$\begin{aligned} dq &= \left(\frac{\partial q}{\partial T}\right)_v dT + \left(\frac{\partial q}{\partial v}\right)_T dv \quad , \\ &= C_v\, dT + T\left(\frac{\partial s}{\partial v}\right)_T dv \quad , \\ &= C_v\, dT + T\left(\frac{\partial P}{\partial T}\right)_v dv \quad . \end{aligned} \tag{20}$$

Equations (19) and (20) give other expressions of the first thermodynamic law:

$$du = C_v\, dT + \left\{ T\left(\frac{\partial P}{\partial T}\right)_v - P \right\} dv \quad , \tag{21}$$

$$dh = C_p\, dT - \left\{ T\left(\frac{\partial v}{\partial T}\right)_p - v \right\} dP \quad . \tag{22}$$

Comparison of the relation:

$$du = \left(\frac{\partial u}{\partial T}\right)_v dT + \left(\frac{\partial u}{\partial v}\right)_T dv \quad ,$$

with the equation (21) gives

$$\left(\frac{\partial u}{\partial v}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_v - P \quad . \tag{23}$$

Similarly we obtain a relation:

$$\left(\frac{\partial h}{\partial P}\right)_T = v - T\left(\frac{\partial v}{\partial T}\right)_p \quad . \tag{24}$$

Using the equation (24) and the relation (1) for v, h and T, we obtain a useful relation:

$$\left(\frac{\partial h}{\partial v}\right)_T = v\left(\frac{\partial P}{\partial v}\right)_T + T\left(\frac{\partial P}{\partial T}\right)_v \quad . \tag{25}$$

A.4.2 Fluid States for 2T Model and Derivatives of State Variables

In a sophisticated two-temperature model, we are interested in the following fluid states:

Subcooled liquid,
Superheated vapor,
Saturated liquid,
Saturated vapor,
Superheated liquid,
Supercooled vapor,
Various mixtures of the above.

The thermodynamic state of fluid as mentioned is determined by the mass and energy conservation equations applied to the mass and energy cells. Four independent variables for the equation of state are basically required to determine the fluid states for each phase under the assumption of equal thermodynamic pressure between phases. Many combinations of four independent variables are possible. The selection of independent variables is not too important, as the inter-relationships among the phase and mixture quantities, and the chain rule for partial differentiation, can be used. Namely, a set of independent variables can be converted to many other possible sets of independent variables.

The balance equations usually include other thermodynamic properties than the selected basic variables. It is favourable that these properties are determined explicitly by the functional relations.

In the present code packages: "STH05G" and "STH05L", the thermodynamic quantities are available in the tabular form with the set of (P, h_g) and (P, h_l) as independent variables. Accordingly it is recommended to include P, h_g and h_l as independent variables in the use of the present code packages.

If, for example, the set of independent variables is (P, α, h_g, h_l),

other thermodynamic properties such as specific volume: v and temperature: T than the four variables can be obtained directly by

$$v_k = v_k\ (P,\ h_k) \tag{26}$$

$$T_k = T_k\ (P,\ h_k) \tag{27}$$

where

$$k = g \text{ or } \ell$$

As noted previously, partial derivatives of other thermodynamic properties (i.e. v_g, v_ℓ, T_g, T_ℓ, etc.) with respect to the basic variables (P, α, h_g, h_ℓ) are required for linearization about a known iteration level. We can obtain Jacobian matrix using the functional relations (26) and (27):

$$\begin{pmatrix} dT_g \\ dT_\ell \\ dv_g \\ dv_\ell \end{pmatrix} = \begin{pmatrix} (\frac{\partial T_g}{\partial P})_{hg} & 0 & (\frac{\partial T_g}{\partial h_g})_P & 0 \\ (\frac{\partial T_\ell}{\partial P})_{h\ell} & 0 & 0 & (\frac{\partial T_\ell}{\partial h_\ell})_P \\ (\frac{\partial v_g}{\partial P})_{hg} & 0 & (\frac{\partial v_g}{\partial h_g})_P & 0 \\ (\frac{\partial v_\ell}{\partial P})_{h\ell} & 0 & 0 & (\frac{\partial v_\ell}{\partial h_\ell}) \end{pmatrix} \begin{pmatrix} dP \\ d\alpha \\ dh_g \\ dh_\ell \end{pmatrix} \tag{28}$$

where non-zero entries of the above matrix can be expressed by the output quantities of "STHO5G" and "STHO5L" as described in Section 4. The output quantities include the following material properties: the coefficient of thermal expansion:

$$\beta \equiv \frac{1}{v} (\frac{\partial v}{\partial T})_P \quad , \tag{29}$$

the isothermal compressibility:

$$\kappa \equiv -\frac{1}{v} (\frac{\partial v}{\partial P})_T \quad , \tag{30}$$

and the specific heat at constant pressure:

$$C_P \equiv (\frac{\partial h}{\partial T})_P \quad . \tag{31}$$

The non-zero entries are now reduced to the forms which contain only the output quantities using general thermodynamic relations described previously:

$$\left(\frac{\partial T_k}{\partial P}\right)_{hx} = -\left(\frac{\partial h_k}{\partial P}\right)_{T_k}\left(\frac{\partial T_k}{\partial h_k}\right)_P \qquad \text{(from the equation (1))},$$

$$= -\left[v_k - T_k\left(\frac{\partial v_k}{\partial T_k}\right)_P\right]\frac{1}{C_{pk}} \qquad \text{(from the equation (24))},$$

$$= \frac{v_k(T_k\beta_k - 1)}{C_{pk}} \quad , \tag{32}$$

$$\left(\frac{\partial T_k}{\partial h_k}\right)_P = \frac{1}{C_{pk}} \quad ,$$

$$\left(\frac{\partial v_k}{\partial P}\right)_{h_k} = -\left(\frac{\partial h_k}{\partial P}\right)_{v_k}\left(\frac{\partial v_k}{\partial h_k}\right)_P \qquad \text{(from the equation (1))} \quad ,$$

$$= -\left(\frac{\partial h_k}{\partial P}\right)_{v_k}\frac{v_k\beta_k}{C_{pk}} \qquad \text{(from the equation (5) and (29))},$$

$$= -\frac{\left(\frac{\partial h_k}{\partial T_k}\right)_{v_k} - \left(\frac{\partial P}{\partial T_k}\right)_{v_k} v_k + \left(\frac{\partial P}{\partial T_k}\right)_{v_k} v_k}{\left(\frac{\partial P}{\partial T_k}\right)_{v_k}} \times \frac{v_k\beta_k}{C_{pk}} \quad ,$$

$$= -\left\{\frac{C_v}{-\left(\frac{\partial v_k}{\partial T_k}\right)_P\left(\frac{\partial P}{\partial v_k}\right)_{T_k}} + v_k\right\} \times \frac{v_k\beta_k}{C_{pk}} \quad ,$$

$$= -\left[\frac{C_{vk}\kappa_k}{\beta_k} + v_k\right]\frac{v_k\beta_k}{C_{pk}} \quad , \tag{33}$$

$$\left(\frac{\partial v_k}{\partial h_k}\right)_P = \left(\frac{\partial v_k}{\partial T_k}\right)_P\left(\frac{\partial T_k}{\partial h_k}\right)_P \quad ,$$

$$= \frac{v_k\beta_k}{C_{pk}} \quad , \tag{34}$$

where

$$k = g \text{ or } \ell \quad ,$$

and C_{vk} is also reduced as follows: the differentiation of the equation (19) with temperature at constant volume gives

$$C_{vk} = C_{pk} - T_k \left(\frac{\partial v_k}{\partial T_k}\right)_P \left(\frac{\partial P}{\partial T_k}\right)_{v_k} \quad ,$$

$$= C_{pk} + T_k \left(\frac{\partial v_k}{\partial T_k}\right)_P \left(\frac{\partial v_k}{\partial T_k}\right)_P \left(\frac{\partial P}{\partial v_k}\right)_{T_k} \qquad \text{(from the equation (1))},$$

$$= C_{pk} - \frac{T_k v_k \beta^2_k}{\kappa} \quad . \tag{35}$$

It is very important to note that the functional relations (26) and (27) can be applied to the metastable states of the phase of water that is present. The derivatives of those functional relations are also available for the metastable states.

If a set of independent variables does not contain P, h_g and h_l which are independent variables of "STH05G" and "STH05L", a conversion of variables is required. Some thermodynamic analysis codes such as RELAP4 adopt a different set of independent variables from those of the steam table packages. A conversion method, for example, will be presented below. A set contains the mass and energy for each phase per mixture unit volume: M_g, M_l, E_g and E_l which are represented by

$$M_g = \alpha / v_g(P, h_g) \quad , \tag{36}$$

$$M_\ell = (1 - \alpha) / v_\ell(P, h_\ell) \quad , \tag{37}$$

$$E_g = M_g \, u_g(P, h_g) \quad , \tag{38}$$

$$E_\ell = M_\ell \, u_\ell(P, h_\ell) \quad . \tag{39}$$

An inter-relationship of mixture quantities gives:

$$M_g \, u_g(P, h_g) + M_\ell \, u_\ell(P, h_\ell) - E_g - E_\ell = 0 \quad . \tag{40}$$

In this example, the balance equations give M_g, M_l, E_g and E_l and all other thermodynamic quantities must be determined with fixing these quantities and using the functional relations: $u_k = u_k(P, h_k)$. The equation (40) can be used to determine P, h_g and h_l. These quantities, however, can not be obtained explicitly from the present code package. Some iteration techniques such as the Newton method is required because M_g, M_l, E_g and E_l are not included as independent variables in the present code packages: "STHO5G" and "STHO5L". Once the P, h_g and h_l are obtained, other quantities such as specific volume and temperature, etc. can be determined directly by the code packages.

The partial derivatives of various thermodynamic properties (i.e., P, α, h_g, h_l, T_g, T_l, u_g, u_l, etc.) with respect to the set (M_g, M_l, E_g, E_l) can be also obtained by using the equation (40) and the functional relations. The form of Jacobian matrix is given by the following:

$$\begin{bmatrix} dP \\ d\alpha \\ dh_g \\ dh_\ell \\ dT_g \\ dT_\ell \\ du_g \\ du_\ell \end{bmatrix} = \begin{bmatrix} (\frac{\partial P}{\partial M_g}), & (\frac{\partial P}{\partial M_\ell}), & (\frac{\partial P}{\partial E_g}), & (\frac{\partial P}{\partial E_\ell}) \\ (\frac{\partial \alpha}{\partial M_g}), & (\frac{\partial \alpha}{\partial M_\ell}), & (\frac{\partial \alpha}{\partial E_g}), & (\frac{\partial \alpha}{\partial E_\ell}) \\ (\frac{\partial h_g}{\partial M_g}), & (\frac{\partial h_g}{\partial M_\ell}), & (\frac{\partial h_g}{\partial E_g}), & (\frac{\partial h_g}{\partial E_\ell}) \\ (\frac{\partial h_\ell}{\partial M_g}), & (\frac{\partial h_\ell}{\partial M_\ell}), & (\frac{\partial h_\ell}{\partial E_g}), & (\frac{\partial h_\ell}{\partial E_\ell}) \\ (\frac{\partial T_g}{\partial M_g}), & (\frac{\partial T_g}{\partial M_\ell}), & (\frac{\partial T_g}{\partial E_g}), & (\frac{\partial T_g}{\partial E_\ell}) \\ (\frac{\partial T_\ell}{\partial M_g}), & (\frac{\partial T_\ell}{\partial M_\ell}), & (\frac{\partial T_\ell}{\partial E_g}), & (\frac{\partial T_\ell}{\partial E_\ell}) \\ (\frac{\partial u_g}{\partial M_g}), & (\frac{\partial u_g}{\partial M_\ell}), & (\frac{\partial u_g}{\partial E_g}), & (\frac{\partial u_g}{\partial E_\ell}) \\ (\frac{\partial u_\ell}{\partial M_g}), & (\frac{\partial u_\ell}{\partial M_\ell}), & (\frac{\partial u_\ell}{\partial E_g}), & (\frac{\partial u_\ell}{\partial E_\ell}) \end{bmatrix} \begin{bmatrix} dM_g \\ dM_\ell \\ dE_g \\ dE_\ell \end{bmatrix} \qquad (41)$$

where all entries can be also reduced to the forms which contain output quantities of the code packages and the set of variables: M_g, M_l, E_g and E_l.

When dependent variables are different from those of "STH05G" and "STH05L", a user must provide some inter-relationships and Jacobian matrix.