

II P-PROPATH:

**Pure Substances and Mixtures
with Fixed Composition**

1. General Features

1.1 FUNCTION SUBPROGRAM REFERENCE

Every P-PROPATH user has to make an initialization process by one of the following two procedures.

1.1.1 Initialization by COMMON VARIABLES

Every user's PROGRAM UNIT which is going to CALL the P-PROPATH FUNCTION SUBPROGRAM should include the following one LINE before the first EXECUTABLE STATEMENT.

```
COMMON/UNIT/KPA, MESS
```

KPA and MESS are reserved as INTEGER VARIABLES. Furthermore, the following two LINES must be placed in the user's PROGRAM UNIT before the first FUNCTION CALL appears.

```
KPA= M  
MESS= N
```

where both M and N are INTEGERS selected by a user.

KPA specifies the units of pressure and temperature for P-PROPATH FUNCTIONS and their ARGUMENTS. Descriptions on the system of units will be found in 1.3 and the relation between the value of M and the units is shown there. When a user wishes to use other units in his/her PROGRAM UNIT later, he/she is supposed to do the same at that place.

MESS specifies whether the message to the erroneous FUNCTION REFERENCE is to be printed out to the standard listing device or not. P-PROPATH does not return any messages when $N = 0$, while it does when $N \neq 0$.

1.1.2 Initialization by SUBROUTINE SUBPROGRAM KPAMES

The alternative method to set the values for KPA and MESS is to make use of SUBROUTINE SUBPROGRAM KPAMES as the following.

```
CALL KPAMES(KPA,MESS)
```

1.2 Operations to Manage Erroneous FUNCTION REFERENCE

A predetermined sequence of operations will occur to process the erroneous FUNCTION REFERENCE when an improper FUNCTION REFERENCE has been done. Erroneous FUNCTION REFERENCES are grouped into 3 levels, with the ascending severity of the user's mistake. (A user has committed a more serious mistake when he/she gets a level 2 ERROR than when a level 1 ERROR occurs)

1.2.1 Level 1 ERROR (Convergence Failure)

The method of iteration, which is built into some of the P-PROPATH FUNCTION SUBPROGRAMs to solve an implicit equation, may not work in some cases where a user has specified an ARGUMENT of FUNCTION very close to the saturation line or the critical point. A level 1 ERROR means P-PROPATH has stopped performing the iteration after the preset maximum number of iteration. Then the P-PROPATH FUNCTION SUBPROGRAM returns him/her an unexpected FUNCTION value and an ERROR message, though the user is not responsible for this type of ERROR,. A level 1 ERROR is processed as shown below.

```
value of FUNCTION returned to the CALLing program: -1.0E+10
output to the standard listing device:
**** NO CONVERGENCE AT (NAME OF FUNCTION CALLED) ****
```

The PROPATH group is working hard to ensure that P-PROPATH FUNCTION SUBPROGRAM will not react with level 1 ERRORS because of poor programming technique. However when a user wants to get a value of a thermophysical property just on the saturation line or at the critical point and not at a point very close to it, he/she should try to CALL another FUNCTION for the states on the saturation line or at the critical point.

1.2.2 Level 2 ERROR (Invalid ARGUMENT(s))

A level 2 ERROR occurs when the ARGUMENT a user transferred to P-PROPATH FUNCTION has failed to drop in the proper range. A level 2 ERROR is processed as shown below.

```
value of FUNCTION returned to the CALLing program: -1.0E+20
output to the standard listing device:
**** OUT OF RANGE AT (NAME OF FUNCTION) FOR (NAME OF SUBSTANCE) WHEN
(FIRST ARGUMENT) AND (SECOND ARGUMENT, if any) ****
```

FUNCTION tables provides the proper range of ARGUMENT(s) for each substance.

1.2.3 Level 3 ERROR (FUNCTION Unavailable)

A user encounters a level 3 ERROR when a P-PROPATH FUNCTION SUBPROGRAM is not available for the substance selected. A level 3 ERROR is processed as shown below.

```
value of FUNCTION returned to the CALLing program: -1.0E+30
output to the standard listing device:
**** FUNCTION (NAME OF FUNCTION CALLED) UNAVAILABLE FOR (NAME OF
SUBSTANCE) ****
```

Function table provides a list of FUNCTION SUBPROGRAMs available for each substance.

1.3 System of Units

All quantities, REAL ARGUMENTs and values of FUNCTION, are in the fundamental SI or in the coherent derived SI with two exceptions. Pressure can be in the unit of Pascal Pa or bar, and temperature in the unit of Kelvin K or degree Celsius °C. Users are allowed to make their own selection on these units by specifying a value to COMMON INTEGER VARIABLE KPA. The procedure to set a value to KPA is described in 1.1, and the relation between the value of KPA and the units of pressure and temperature is shown in the table below. The temperature is based on the International Practical Temperature Scale 1968, IPTS-1968 or International Temperature Scale, ITS-1990.

Table II-1-1 Units of Pressure and Temperature Specified by KPA

KPA	unit of pressure	unit of temperature
0	Pa	K
1	bar	°C
2	bar	K
3	Pa	°C
others	Pa	K

1.4 Reserved NAMES

P-PROPATH uses a lot of NAMES, listed below, for its own purpose. These are the NAMES of FUNCTION SUBPROGRAMS to which a user can access directly, KPA, the first COMMON INTEGER VARIABLE, to specify the units of pressure and temperature, and MESS, the second COMMON INTEGER VARIABLE, to allow or suppress the listing of error messages. These are supposed to appear in the user's PROGRAM UNIT only when they assume their original meaning. A, B, C, ... are the first LETTERS in the NAMES listed in the same line.

NAMES of FUNCTION SUBPROGRAMS:

A : AIPPT, AJTPT, AKPD, AKPDD, AKPT, AKTD, AKTDD, ALAPP, ALAPT,
 : ALHP, ALHT, ALMPD, ALMPDD, ALMPT, ALMTD, ALMTDD, AMUPD, AMUPDD,
 : AMUPT, AMUTD, AMUTDD
 B : BPPT, BSPT, BTPT, BVPT
 C : CPPD, CPPDD, CPPT, CPTD, CRP, CPTDD, CVPD, CVPDD, CVPT, CVTD, CVTDD
 E : EPSPD, EPSPDD, EPSPT, EPSTD, EPSTDD
 F : FC
 G : GAMPD, GAMPDD, GAMPT, GAMTD, GAMTDD
 H : HPD, HPDD, HPS, HPT, HPX, HTD, HTDD, HTX
 I : IDENTF
 P : PLDT, PMLT, PRPD, PRPDD, PRPT, PRTD, PRTDD, PST, PSTD, PSTDD
 S : SIGP, SIGT, SPD, SPDD, SPT, SPX, STD, STDD, STX
 T : T68, T90, TLDP, TMLP, TPH, TPH2, TPS, TPS2, TPSEUP, TPV, TRPL,
 : TSBP, TSP, TSPD, TSPDD
 U : UPD, UPDD, UPS, UPT, UPX, UTD, UTDD, UTX
 V : VPD, VPDD, VPS, VPT, VPX, VTD, VTDD, VTX
 W : WPD, WPDD, WPT, WTD, WTDD
 X : XPH, XPS, XPU, XPV, XTH, XTS, XTU, XTV

NAMES of COMMON INTEGER VARIABLEs:

K : KPA
 M : MESS

1.5 Naming Convention of FUNCTION SUBPROGRAM

The NAMES of FUNCTION SUBPROGRAM have been allocated in a regular pattern. This will help a user to remember them. The first one to six LETTERS stand for the kinds of the thermophysical properties. These are, in alphabetical order,

“AIP”	=ion product
“AJT”	=Joul-Thomson coefficient
“AK”	=isentropic exponent
“ALAP”	=Laplace coefficient
“ALH”	=latent heat of vaporization
“ALM”	=thermal conductivity
“AMU”	=coefficient of viscosity
“BP”	=volmetric coefficient of expansion
“BS”	=isentropic compressibility
“BT”	=isothermal compressibility
“BV”	=pressure coefficient
“CP”	=isobaric specific heat
“CRP”	=critical constants
“CV”	=isochoric specific heat
“EPS”	=static dielectric constant
“FC”	=fundamental constants
“GAM”	=ratio of specific heats
“H”	=specific enthalpy
“IDENTF”	=name of substance or version number
“PLD”	=pressure on λ line
“PML”	=pressure on melting line
“PR”	=Prandtl number
“PS”	=saturation pressure
“S”	=specific entropy
“SIG”	=surface tension
“T”	=temperature
“TLD”	=temperature on λ line
“TML”	=temperature on melting line
“TPSEU”	=pseudo boiling temperature
“TRPL”	=property at the triple point
“TS”	=saturation temperature
“U”	=specific internal energy
“V”	=specific volume
“W”	=velocity of sound
“X”	=dryness fraction of wet vapor

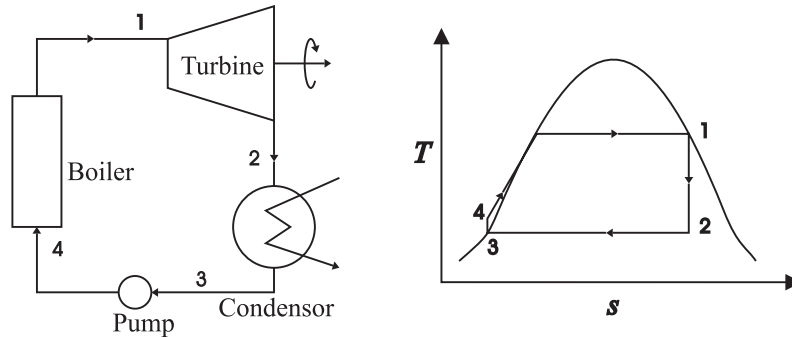
“A” at the top of the first 6 of these has been attached to avoid the DEFAULT IMPLIED TYPING characteristic of FORTRAN language.

After these one to six LETTERS mentioned above, there come the LETTER(s) reminding users of the pertinent ARGUMENT(s). These are made of one or two LETTERS, and in the latter case the order of the two LETTERS coincides with the order of the ARGUMENTS which they stand for in the parentheses () of FUNCTION symbol. They are “H”= specific enthalpy, “P”= pressure, “S”= specific entropy, “T”= temperature, “U”= specific internal energy, “V”= specific volume, and “X”= dryness fraction of wet vapor. However no LETTER follows after “CRP”, “FC”, “IDENTF” and “TRPL”. In these four FUNCTION SUBPROGRAMS, they are argued by a CHARACTER. For the case of “CRP” and “TRPL”, one of ‘H’, ‘P’, ‘S’, ‘T’, and ‘V’ is the possible CHARACTER CONSTANT, and the value of the FUNCTION is specific enthalpy, pressure, specific entropy, temperature or specific volume in the same order. For “FC”, either ‘M’ or ‘R’ is the possible, and the value of the FUNCTION is molecular weight or gas constant. Finally, for “IDENTF” one of ‘C’, ‘S’ or ‘V’ is possible, and the molecular formula, the name of substance or the version number of the package is provided as a CHARACTER value.

Lastly the NAME of FUNCTION SUBPROGRAM ends with “D” and “DD” standing for the saturated liquid and the dry saturated vapor, respectively. These conform to the Japanese and German conventions “ ’ ” and “ ” ” in the thermodynamic literature. In English literature, they are symbolized as “ f ” and “ g ”, respectively.

1.6 An Example of User's PROGRAM UNIT

[**Example**] A reversible Rankine cycle works between a higher pressure of 10 MPa and a lower pressure of 5 kPa (see figure). Find the cycle effectiveness, the thermal efficiency, the work ratio and the steam rate. Assume a reference temperature of 25°C.



Reversible Rankine Cycle

Sample Program

```

1 *****
2 *
3 *   SAMPLE PROGRAM FOR /PROPATH/ USERS   *
4 *
5 *   EXAMPLE FROM       NISHIKAWA AND ITO, *
6 *                       OHYOH NETSURIKIGAKU, *
7 *                       CORONA SHA, TOKYO, *
8 *                       1983                *
9 *
10 *****
11 *
12 ***** EX.11.4 ON PAGE 306, CYCLE EFFICIENCY, WORK RATIO, *****
13 ***** AND STEAM RATE FOR RANKINE CYCLE *****
14 *
15     REAL*4 L,L0,LTO,LPO
16     COMMON/UNIT/KPA, MESS
17     KPA=1
18     MESS=1
19     P1=100.0
20     P2=0.05
21     T0=298.15
22     H1=HPDD(P1)
23     S1=SPDD(P1)
24     H3=HPD(P2)
25     R=ALHP(P2)
26     S3=SPD(P2)
27     X=XPS(P2,S1)
28     H2=H3+X*R
29     T4=TPS(P1,S3)
30     H4=HPT(P1,T4)
31     LTO=H1-H2
32     LPO=H4-H3
33     L0=LTO-LPO
34     QB0=H1-H4
35     L=L0/LTO

```

```

36     ETA=L0/QB0
37     G0=3600.0/L0*1000.
38     GTO=3600.0/LTO*1000.
39     PSI1=H1-T0*S1
40     PSI4=H4-T0*S3
41     ETAC=L0/(PSI1-PSI4)
42     WRITE(6,*)'***** SAMPLE PROGRAM FOR /PROPATH/ USERS *****'
43     WRITE(6,*)'   CYCLE EFFICIENCY           ETA =',ETA
44     WRITE(6,*)'   WORK RATIO                 L0  =',L
45     WRITE(6,*)'   STEAM RATE PER NET POWER   G0  =',
46     &   GO,' (KG/KWH) '
47     WRITE(6,*)'   STEAM RATE PER TURBINE POWER   GTO =',
48     &   GTO,' (KG/KWH) '
49     WRITE(6,*)'   CYCLE EFFECTIVENESS         EATC=',ETAC
50     STOP
51     END

```

Output

```

***** SAMPLE PROGRAM FOR /PROPATH/ USERS *****
CYCLE EFFICIENCY           ETA =0.38983846
WORK RATIO                 L0  =0.99013019
STEAM RATE PER NET POWER   G0  =3.5793953 (KG/KWH)
STEAM RATE PER TURBINE POWER   GTO =3.5440674 (KG/KWH)
CYCLE EFFECTIVENESS         ETAC=0.96117246

```


6: PST, ALAPT, ALMTD, ALMTDD, AMUTD, AMUTDD	20: XTV
7: CPTD, CPTDD, CVTDD, GAMTDD, PRTD, PRTDD	21: HTX, STX, UTX, VTX
SIGT	22: CRP, FC, TRPL
8: PST, PSTD, PSTDD, PLDT, PMLT, PSBT	23: T90, T68
9: VPT, HPT, SPT, UPT	
10: ALMPT, AMUPT, CPPT, CVPT, GAMPT, PRPT	
11: AKPT, AJTPT, AIPPT, BPPT, BSPT, BTPT	99: Change System of Unit
BVPT, EPSPT, WPT	0: Quit

Input No. : 99

No.	Unit	(Current)
1 --->	Pressure	[Pa]
2 --->	Temperature	[K]
3 --->	Energy	[J/kg]
	Entropy and Sp. Heat	[J/(kg*K)]
4 --->	Specific Volume	[m**3/kg]
5 --->	Thermal Conductivity	[W/(m*K)]
6 --->	Viscosity	[Pa*s]
7 --->	Surface Tension	[N/m]
8 --->	Laplace Coefficient	[m]
9 --->	Sonic Velocity	[m/s]
10 --->	Joul-Thomson Coef.	[K/Pa]
0 --->	Return to the Function Menu	

Input No. : 1

Unit for Pressure

1 --->	[Pa]
2 --->	[kPa]
3 --->	[MPa]
4 --->	[bar]
5 --->	[ata]
6 --->	[atm]
7 --->	[mmHg]
8 --->	[lb/in**2]
9 --->	[lb/ft**2]

Input No. : 3

No.	Unit	(Current)
1 --->	Pressure	[MPa]
2 --->	Temperature	[K]
3 --->	Energy	[J/kg]
	Entropy and Sp. Heat	[J/(kg*K)]
4 --->	Specific Volume	[m**3/kg]
5 --->	Thermal Conductivity	[W/(m*K)]
6 --->	Viscosity	[Pa*s]
7 --->	Surface Tension	[N/m]
8 --->	Laplace Coefficient	[m]
9 --->	Sonic Velocity	[m/s]
10 --->	Joul-Thomson Coef.	[K/Pa]
0 --->	Return to the Function Menu	

Input No. : 2

Unit for Temperature

1 --->	[K]
2 --->	[C]
3 --->	[F]
4 --->	[R]

Input No. : 2

No.	Unit	(Current)
1 --->	Pressure	[MPa]

```

2 ---> Temperature      [C]
3 ---> Energy            [J/kg]
      Entropy and Sp. Heat [J/(kg*K)]
4 ---> Specific Volume  [m**3/kg]
5 ---> Thermal Conductivity [W/(m*K)]
6 ---> Viscosity        [Pa*s]
7 ---> Surface Tension  [N/m]
8 ---> Laplace Coefficient [m]
9 ---> Sonic Velocity   [m/s]
10 ---> Joule-Thomson Coef. [K/Pa]
0 ---> Return to the Function Menu

```

Input No. : 0

```

=====
|          SS: An Application Program for PROPATH Providing          |
| Thermophysical Properties of WATER(IFC 1967) (H2O) VER.10.1      |
=====

```

No.	PROPATH Functions	No.	PROPATH Functions
1:	TSP, VPD, VPDD, HPD, HPDD, SPD, SPDD UPD, UPDD, ALHP	12:	TPH, XPH
2:	TSP, ALAPP, ALMPD, ALMPDD, AMUPD, AMUPDD	13:	HPS, TPS, UPS, VPS, XPS
3:	CPPD, CPPDD, CVPDD, GAMPDD, PRPD, PRPDD SIGP	14:	XPU
4:	TSP, TSPD, TSPDD, TLDP, TMLP, TPSEUP, TSBP	15:	TPV, XPV
5:	PST, VTD, VTDD, HTD, HTDD, STD, STDD UTD, UTDD, ALHT	16:	HPX, SPX, UPX, VPX
6:	PST, ALAPT, ALMTD, ALMTDD, AMUTD, AMUTDD	17:	XTH
7:	CPTD, CPTDD, CVTDD, GAMTDD, PRTD, PRTDD SIGT	18:	XTS
8:	PST, PSTD, PSTDD, PLDT, PMLT, PSBT	19:	XTU
9:	VPT, HPT, SPT, UPT	20:	XTV
10:	ALMPT, AMUPT, CPPT, CVPT, GAMPT, PRPT	21:	HTX, STX, UTX, VTX
11:	AKPT, AJTPT, AIPPT, BPPT, BSPT, BTPT BVPT, EPSPT, WPT	22:	CRP, FC, TRPL
		23:	T90, T68
		99:	Change System of Unit
		0:	Quit

Input No. : 9

Calculation of VPT, HPT, SPT, UPT

```

=====
Input P[MPa] and T[C] ( P<0 : Quit) : 20.0,450.0
      P= 2.000000E+01 [MPa]          T= 4.500000E+02 [C]
      VPT= 1.270676E-02 [m**3/kg]    HPT= 3.064273E+06 [J/kg]
      SPT= 5.908902E+03 [J/(kg*K)]   UPT= 2.810137E+06 [J/kg]

```

Input P[MPa] and T[C] (P<0 : Quit) : -1,0

```

=====
|          SS: An Application Program for PROPATH Providing          |
| Thermophysical Properties of WATER(IFC 1967) (H2O) VER.10.1      |
=====

```

No.	PROPATH Functions	No.	PROPATH Functions
1:	TSP, VPD, VPDD, HPD, HPDD, SPD, SPDD UPD, UPDD, ALHP	12:	TPH, XPH
2:	TSP, ALAPP, ALMPD, ALMPDD, AMUPD, AMUPDD	13:	HPS, TPS, UPS, VPS, XPS
3:	CPPD, CPPDD, CVPDD, GAMPDD, PRPD, PRPDD SIGP	14:	XPU
4:	TSP, TSPD, TSPDD, TLDP, TMLP, TPSEUP, TSBP	15:	TPV, XPV
5:	PST, VTD, VTDD, HTD, HTDD, STD, STDD UTD, UTDD, ALHT	16:	HPX, SPX, UPX, VPX
6:	PST, ALAPT, ALMTD, ALMTDD, AMUTD, AMUTDD	17:	XTH
7:	CPTD, CPTDD, CVTDD, GAMTDD, PRTD, PRTDD SIGT	18:	XTS
8:	PST, PSTD, PSTDD, PLDT, PMLT, PSBT	19:	XTU
9:	VPT, HPT, SPT, UPT	20:	XTV
10:	ALMPT, AMUPT, CPPT, CVPT, GAMPT, PRPT	21:	HTX, STX, UTX, VTX
11:	AKPT, AJTPT, AIPPT, BPPT, BSPT, BTPT BVPT, EPSPT, WPT	22:	CRP, FC, TRPL
		23:	T90, T68
		99:	Change System of Unit
		0:	Quit

Input No. : 22

Calculation of CRP, FC, TRPL

=====

Critical Constants

H= 2.107400E+06 [J/kg] P= 2.212000E+01 [MPa]
 S= 4.442860E+03 [J/(kg*K)] T= 3.741500E+02 [C]
 V= 3.170000E-03 [m**3/kg]

Fundamental Constants

M= 1.801530E+01 [-] R= 4.615100E+02 [J/(kg*K)]

Triple Point

P= 6.112000E-04 [MPa] T= 1.000977E-02 [C]

-- Hit RETURN Key to Function Menu---

=====

| SS: An Application Program for PROPATH Providing |
 | Thermophysical Properties of WATER(IFC 1967) (H2O) VER.10.1 |
 |=====|

No.	PROPATH Functions	No.	PROPATH Functions
1:	TSP, VPD, VPDD, HPD, HPDD, SPD, SPDD	12:	TPH, XPH
	UPD, UPDD, ALHP	13:	HPS, TPS, UPS, VPS, XPS
2:	TSP, ALAPP, ALMPD, ALMPDD, AMUPD, AMUPDD	14:	XPU
3:	CPPD, CPPDD, CVPDD, GAMPDD, PRPD, PRPDD	15:	TPV, XPV
	SIGP	16:	HPX, SPX, UPX, VPX
4:	TSP, TSPD, TSPDD, TLDP, TMLP, TPSEUP, TSBP	17:	XTH
5:	PST, VTD, VTDD, HTD, HTDD, STD, STDD	18:	XTS
	UTD, UTDD, ALHT	19:	XTU
6:	PST, ALAPT, ALMTD, ALMTDD, AMUTD, AMUTDD	20:	XTV
7:	CPTD, CPTDD, CVTDD, GAMTDD, PRTD, PRTDD	21:	HTX, STX, UTX, VTX
	SIGT	22:	CRP, FC, TRPL
8:	PST, PSTD, PSTDD, PLDT, PMLT, PSBT	23:	T90, T68
9:	VPT, HPT, SPT, UPT		
10:	ALMPT, AMUPT, CPPT, CVPT, GAMPT, PRPT		
11:	AKPT, AJTPT, AIPPT, BPPT, BSPT, BTPT	99:	Change System of Unit
	BVPT, EPSPT, WPT	0:	Quit

=====

Input No. : 0

***** See You Again ! *****

Stop - Program terminated.