

## **IV M-PROPATH: Binary Mixtures**

Binary mixtures in part IV stand for those that have been formulated as binary mixtures by their own formulations.

## 1. General Features

### 1.1 SUBPROGRAM REFERENCE

Every M-PROPATH user has to make the initiation process by writing the following 2 lines before the first REFERENCE to a M-PROPATH SUBPROGRAM (FUNCTION SUBPROGRAM or SUBROUTINE SUBPROGRAM) in the MAIN PROGRAM. If a user happens to want to use other settings in other places of his/her PROGRAM UNIT, he/she is supposed to do a similar at those places.

```
CALL KPAMES(value of KPA, value of MESS)
CALL STNKAS(value of KSTAN, value of KAS)
```

The arguments of these SUBROUTINE SUBPROGRAMs specify the system of units, reference values of enthalpy and entropy and necessity of listing error messages to erroneous SUBPROGRAM REFERENCES on the standard output device. All arguments in these SUBROUTINE SUBPROGRAMs are INTEGERS. KPA specifies the units of pressure and temperature, and KAS unit of the amount of substance. KSTAN selects the reference values of enthalpy and entropy. The relation between KPA and the units of pressure and temperature and that between KAS and the unit of amount of substance are shown in 1.3. M-PROPATH does not return any messages when MESS=0, while it does when MESS≠0. KSTAN differs from one mixture to another, and is described in the section of each mixture.

## 1.2 Operations to Manage Erroneous SUBPROGRAM REFERENCE

A predetermined sequence of operations will occur to process an erroneous SUBPROGRAM REFERENCE when an improper SUBPROGRAM REFERENCE has been done. Erroneous SUBPROGRAM REFERENCEs are grouped into 2 levels, with the ascending severity of user's mistake. A user has committed a more serious mistake when a level 2 ERROR occurs than when level 1 ERROR does.

### 1.2.1 Level 1 ERROR (Convergence Failure)

The method of iterations built in to some of the M-PROPATH SUBPROGRAMs to solve implicit relations will not work somehow from time to time. M-PROPATH stops further iterations after executing the preset number of iterations. Though the user is not responsible for level 1 ERROR, the M-PROPATH detects this type of ERROR time to time, unfortunately.

A level 1 ERROR is processed as below.

#### FUNCTION SUBPROGRAM

value of REAL FUNCTION returned to the CALLing program :  $-1.0E+10$   
 value of INTEGER FUNCTION returned to the CALLing Program :  $-1$   
 output to the standard output device :  
       \*\*\*\* NO CONVERGENCE AT (NAME OF FUNCTION CALLED) \*\*\*\*

#### SUBROUTINE SUBPROGRAM

value of error detection cord :  $-1$   
 output to the standard output device :  
       \*\*\*\* NO CONVERGENCE AT (NAME OF SUBROUTINE CALLED) \*\*\*\*

### 1.2.2 Level 2 ERROR (Invalid ARGUMENT(s))

A level 2 ERROR will occur when the ARGUMENT(s) a user transferred to M-PROPATH SUBPROGRAM from his/her MAIN PROGRAM fail to drop in the proper range.

A level 2 ERROR is processed as below.

#### FUNCTION SUBPROGRAM

value of REAL FUNCTION returned to the CALLing program :  $-1.0E+20$   
 value of INTEGER FUNCTION returned to the CALLing Program :  $-2$   
 output to the standard output device :  
       \*\*\*\* OUT OF RANGE AT (NAME OF FUNCTION CALLED) \*\*\*\*

#### SUBROUTINE SUBPROGRAM

value of error detection cord :  $-2$   
 output to the standard output device :  
       \*\*\*\* OUT OF RANGE AT (NAME OF SUBROUTINE CALLED) \*\*\*\*

### 1.3 System of Units and Reference Value of Enthalpy and Entropy

All REAL quantities are in the fundamental SI or in the coherent derived SI with three exceptions. Pressure can be in the unit of Pascal Pa or bar, temperature in the unit of Kelvin K or degree Celsius °C. These depend on the value of INTEGER KPA when a user referred the SUBROUTINE SUBPROGRAM KPAMES(KPA, MESS) shown in 1.1. The amount of substance can be in the unit of kilomole kmol or kilogram kg. INTEGER KAS in the SUBROUTINE SUBPROGRAM STNKAS(KSTAN, KAS) in 1.1 switches this. These go as shown in the table below. The INTEGER KSTAN in the SUBROUTINE SUBPROGRAM STNKAS(KSTAN, KAS) controls the reference values of enthalpy and entropy and is explained for each specific mixture, since they differ from one mixture to another.

Table IV-1.3-1 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

Table IV-1.3-2 Amount of Substance Specified by KAS

KAS	amount of substance
0	kmol
1	kg
others	kmol

## 1.4 Reserved NAMES

M-PROPATH uses a lot of NAMES, listed below, for its own purpose. These are the NAMES of SUBPROGRAMS and NAMED COMMON BLOCK to which a user can access directly and NAMES of SUBPROGRAM headed by "FMF" which an user cannot access. A user is supposed to use the NAMES of SUBPROGRAM and COMMON BLOCK only when he/she does so in the original meaning. The letters in the first column are the first LETTERS in the NAMES listed in the same line.

### Name of COMMON BLOCK, FUNCTION and SUBROUTINE

**F** FCM, FMF\*\*\*\* , COMMON /FMFC/  
**I** IDENTM, IPHASE  
**K** KPAMES  
**P** PSTM  
**S** STNKAS, SUBM, SUBMIX, SUBPB, SUBPD, SUBPST, SUBPUR, SUBTB, SUBTD,  
SUBTSP, SUBXY  
**T** T68, T90, TSPM  
**U** COMMON /UNIT/

## 1.5 Terminology, Symbols and Compositions

The component with lower critical temperature is to be called as the first component. A composition is supposed to stand for the mole fraction or the mass fraction of the first component. The symbolic distinction of the compositions between the two phases and that between two saturation temperatures are done as shown below.

total composition Z	:	composition of mixture as a whole
composition at liquid phase X	:	liquid composition at vapor-liquid equilibrium
composition at vapor phase Y	:	vapor composition at vapor-liquid equilibrium
temperature at dew point	:	The lowest temperature of vapor for given pressure and Z
temperature at bubble point	:	The highest temperature of liquid for given pressure and Z
pressure at dew point	:	The highest pressure of vapor for given temperature and Z
pressure at bubble point	:	The lowest pressure of liquid for given temperature and Z

## 1.6 The NAME of FUNCTION and SUBROUTINE SUBPROGRAMS

NAMES of FUNCTIONS and SUBROUTINES are shown below and the full description of these SUBPROGRAMS is given in 1.7. Some of these SUBPROGRAMS have not been prepared in each equation shown in 2. and after. These are listed there for each equation.

### 1.6.1 FUNCTION

#### REAL valued FUNCTION (conversion of temperature scale)

T68 = conversion from ITS-1990 to IPTS-1968  
T90 = conversion from IPTS-1968 to ITS-1990

#### REAL valued FUNCTION (pure component)

FCM = fundamental constants of pure components  
PSTM = vapor pressure of pure components  
TSPM = saturation temperature of pure components

#### REAL valued FUNCTION (mixture)

AKG = mole fraction to mass fraction conversion  
AKMOL = mass fraction to mole fraction conversion

#### INTEGER valued FUNCTION

IPHASE = distinction between phases of mixture

#### CHARACTER valued FUNCTION

IDENTM = name of pure components and version number

### 1.6.2 SUBROUTINE

#### initialization

KPAMES/STNKAS = See 1.1

#### pure component

SUBPST = saturation properties of pure components (temperature input)  
SUBPUR = single phase properties of pure component  
SUBTSP = saturation properties of pure components (pressure input)

#### mixture

SUBPB = bubble point pressure and other properties of mixture (temperature and X input)  
SUBPD = dew point pressure and other properties of mixture (temperature and Y input)  
SUBTB = bubble point temperature and other properties of mixture (pressure and X input)  
SUBTD = dew point temperature and other properties of mixture (pressure and Y input)  
SUBM = adiabatic and isobaric mixing of two streams  
SUBMIX = properties of mixture  
SUBXY = properties of mixture at VLE  
SUBMXH = isobaric mixing of two mixtures with different composition, enthalpy input  
SUBMXT = isobaric mixing of two mixtures with different composition, temperature input

## 1.7 Descriptions of FUNCTIONS and SUBROUTINES

Shown in alphabetical order of NAMES.

### AKG

REAL FUNCTION **AKG(Z)** : mole fraction to mass fraction conversion

REAL Z : mole fraction [kmol/kmol]

REAL AKG : mass fraction [kg/kg]

### AKMOL

REAL FUNCTION **AKMOL(Z)** : mass fraction to mole fraction conversion

REAL Z : mass fraction [kg/kg]

REAL AKMOL : mole fraction [kmol/kmol]

### FCM

REAL FUNCTION **FCM(I,A)** : fundamental constants of pure components

INTEGER I : component

1 : first component

2 : second component

CHARACTER\*1 A : kind of fundamental constants of pure components

'M' : molar mass [kg/kmol]

'R' : gas constant [J/(kg·K)]

'T' : critical temperature [K], [°C]

'P' : critical pressure [Pa], [bar]

'V' : critical volume [m<sup>3</sup>/kmol], [m<sup>3</sup>/kg]

'E' : acentric factor [-]

### IDENTM

CHARACTER\*40 FUNCTION **IDENTM(I,A)** : name of pure component and version number

INTEGER I : component

1 : first component

2 : second component

CHARACTER\*1 A : kind of characters returned

'C' : molecular formula

'S' : name of substance

'V' : version number

### IPHASE

INTEGER FUNCTION **IPHASE(T,P,Z)** : distinction between phases of mixture

REAL T : temperature [K], [°C]

REAL P : pressure [Pa], [bar]

REAL Z : composition [kmol/kmol], [kg/kg]

value of IPHASE

1 : liquid phase

2 : two phase

3 : gas phase

- 4 : super critical
- 1 : Convergence failure
- 2 : invalid ARGUMENT(s)

**KPAMES**

SUBROUTINE **KPAMES(KPA,MESS)**

See 1.1

**PSTM**

REAL FUNCTION **PSTM(I,T)** : saturation pressure of pure component

- INTEGER I : component
  - 1 : first component
  - 2 : second component
- REAL T : temperature [K] , [°C]
- REAL PSTM : saturation pressure [Pa], [bar]

**STNKAS**

SUBROUTINE **STNKAS(KSTAN,KAS)**

See 1.1

**SUBMIX**

SUBROUTINE **SUBMIX(I,J,T,P,Z,V,H,S)** : properties of mixture

- INTEGER I : type of problem(input)
  - 1 : inputs (T,P,Z) → outputs (V,H,S)
  - 2 : inputs (P,Z,H) → outputs (T,V,S)
  - 3 : inputs (P,Z,S) → outputs (T,V,H)
  - 4 : inputs (P,Z,V) → outputs (T,H,S)
- INTEGER J : error detection code
  - 1 : convergence failure
  - 2 : invalid ARGUMENT(s)
- REAL T : temperature [K] , [°C]
- REAL P : pressure [Pa] , [bar]
- REAL Z : total composition [kmol/kmol] , [kg/kg]
- REAL V : volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]
- REAL H : enthalpy [J/kmol] , [J/kg]
- REAL S : entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBMXH**

SUBROUTINE **SUBMXH(J,T,P,ZA,ZB,Z,V,HA,HB,H,S,W)** : isobaric mixing of two mixtures with different compositions, enthalpy input

input

- REAL P : pressure [Pa] , [bar]
- REAL ZA : total composition of A [kmol/kmol] , [kg/kg]
- REAL ZB : total composition of B [kmol/kmol] , [kg/kg]
- REAL HA : enthalpy of A [J/kmol] , [J/kg]
- REAL HB : enthalpy of B [J/kmol] , [J/kg]
- REAL W : Fraction of A in Mixing [kmol/kmol] , [kg/kg]

output

- INTEGER J : error detection code
  - 1 : convergence failure
  - 2 : invalid ARGUMENT(s)
- REAL T : temperature after mixing [K] , [°C]
- REAL Z : total composition after mixing [kmol/kmol] , [kg/kg]
- REAL V : volume after mixing [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]

REAL H : enthalpy after mixing [J/kmol] , [J/kg]  
 REAL S : entropy after mixing [J/(kmol·K)] , [J/(kg·K)]

**SUBMXT**

SUBROUTINE **SUBMXT(J,T,P,ZA,ZB,Z,V,TA,TB,H,S,W)** : isobaric mixing of two mixtures with different compositions, temperature input

input

REAL P : pressure [Pa] , [bar]  
 REAL ZA : total composition of A [kmol/kmol] , [kg/kg]  
 REAL ZB : total composition of B [kmol/kmol] , [kg/kg]  
 REAL TA : temperature of A [K] , [°C]  
 REAL TB : temperature of B [K] , [°C]  
 REAL W : Fraction of A in Mixing [kmol/kmol] , [kg/kg]

output

INTEGER J : error detection code  
 -1 : convergence failure  
 -2 : invalid ARGUMENT(s)  
 REAL T : temperature after mixing [K] , [°C]  
 REAL Z : total composition after mixing [kmol/kmol] , [kg/kg]  
 REAL V : volume after mixing [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL H : enthalpy after mixing [J/kmol] , [J/kg]  
 REAL S : entropy after mixing [J/(kmol·K)] , [J/(kg·K)]

**SUBPB**

SUBROUTINE **SUBPB(J,T,P,X,V,H,S)**

: bubble point pressure and other properties of mixture (temperature and X input)

input

REAL T : temperature [K] , [°C]  
 REAL X : composition [kmol/kmol] , [kg/kg]

output

INTEGER J : error detection code  
 -1 : convergence failure  
 -2 : invalid ARGUMENT(s)  
 REAL P : bubble point pressure [Pa] , [bar]  
 REAL V : bubble point volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL H : bubble point enthalpy [J/kmol] , [J/kg]  
 REAL S : bubble point entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBPD**

SUBROUTINE **SUBPD(J,T,P,Y,V,H,S)**

: dew point pressure and other properties of mixture (temperature and Y input)

input

REAL T : temperature [K] , [°C]  
 REAL Y : composition [kmol/kmol] , [kg/kg]

output

INTEGER J : error detection code  
 -1 : convergence failure  
 -2 : invalid ARGUMENT(s)  
 REAL P : dew point pressure [Pa] , [bar]  
 REAL V : dew point volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL H : dew point enthalpy [J/kmol] , [J/kg]  
 REAL S : dew point entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBPST**

**SUBROUTINE SUBPST(I,J,T,PS,VL,VV,HL,HV,SL,SV)**

: saturation properties of pure component (temperature input)

input

INTEGER I : component  
           1 : first component  
           2 : second component  
 REAL T : temperature [K] , [°C]

output

INTEGER J : error detection code  
           -1 : convergence failure  
           -2 : invalid ARGUMENT(s)  
 REAL PS : saturation pressure [Pa] , [bar]  
 REAL VL : liquid volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL VV : vapor volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL HL : liquid enthalpy [J/kmol] , [J/kg]  
 REAL HV : vapor enthalpy [J/kmol] , [J/kg]  
 REAL SL : liquid entropy [J/(kmol·K)] , [J/(kg·K)]  
 REAL SV : vapor entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBPUR**

**SUBROUTINE SUBPUR(I,J,T,P,V,H,S)** : single phase properties of pure component

input

INTEGER I : component  
           1 : first component  
           2 : second component  
 REAL T : temperature [K] , [°C]  
 REAL P : pressure [Pa] , [bar]

output

output are those of saturated liquid, when temperature-pressure is on saturation line

INTEGER J : error detection code  
           -1 : convergence failure  
           -2 : invalid ARGUMENT(s)  
 REAL V : volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL H : enthalpy [J/kmol] , [J/kg]  
 REAL S : entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBTB**

**SUBROUTINE SUBTB(J,T,P,X,V,H,S)**

: bubble point temperature and other properties of mixture (pressure and X input)

input

REAL P : pressure [Pa] , [bar]  
 REAL X : composition [kmol/kmol] , [kg/kg]

output

INTEGER J : error detection code  
           -1 : convergence failure  
           -2 : invalid ARGUMENT(s)  
 REAL T : bubble point temperature [K] , [°C]  
 REAL V : bubble point volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL H : bubble point enthalpy [J/kmol] , [J/kg]  
 REAL S : bubble point entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBTD**

**SUBROUTINE SUBTD(J,T,P,Y,V,H,S)**

: dew point temperature and other properties of mixture (pressure and Y input)

input

REAL P : pressure [Pa] , [bar]  
 REAL Y : composition [kmol/kmol] , [kg/kg]

output

INTEGER J : error detection code  
 -1 : convergence failure  
 -2 : invalid ARGUMENT(s)  
 REAL T : dew point temperature[K] , [°C]  
 REAL V : dew point volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL H : dew point enthalpy[J/kmol] , [J/kg]  
 REAL S : dew point entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBTSP**

SUBROUTINE **SUBTSP(I,J,TS,P,VL,VV,HL,HV,SL,SV)**  
 : saturation properties of pure component (pressure input)

input

INTEGER I : component  
 1 : first component  
 2 : second component  
 REAL P : pressure [Pa] , [bar]

output

INTEGER J : error detection code  
 -1 : convergence failure  
 -2 : invalid ARGUMENT(s)  
 REAL TS : temperature [K] , [°C]  
 REAL VL : liquid volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL VV : vapor volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL HL : liquid enthalpy [J/kmol] , [J/kg]  
 REAL HV : vapor enthalpy [J/kmol] , [J/kg]  
 REAL SL : liquid entropy [J/(kmol·K)] , [J/(kg·K)]  
 REAL SV : vapor entropy [J/(kmol·K)] , [J/(kg·K)]

**SUBXY**

SUBROUTINE **SUBXY(J,T,P,X,Y,VL,VV,HL,HV,SL,SV)** :properties of mixture at VLE

input

REAL T : temperature [K] , [°C]  
 REAL P : pressure [Pa] , [bar]

output

INTEGER J : error detection code  
 -1 : convergence failure  
 -2 : invalid ARGUMENT(s)  
 REAL X : composition of liquid X [kmol/kmol] , [kg/kg]  
 REAL Y : composition of vapor Y [kmol/kmol] , [kg/kg]  
 REAL VL : liquid volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL VV : vapor volume [m<sup>3</sup>/kmol] , [m<sup>3</sup>/kg]  
 REAL HL : liquid enthalpy [J/kmol] , [J/kg]  
 REAL HV : vapor enthalpy [J/kmol] , [J/kg]  
 REAL SL : liquid entropy [J/(kmol·K)] , [J/(kg·K)]  
 REAL SV : vapor entropy [J/(kmol·K)] , [J/(kg·K)]

**TSPM**

REAL FUNCTION **TSPM(I,P)** saturation temperature of pure components

INTEGER I : component  
 1 : first component  
 2 : second component

REAL P : pressure of pure component [Pa] , [bar]  
REAL TSPM : saturation temperature [K], [°C]