

IK - CAPE - PPDx

Physical Property Data EXchange - Neutral File Format

VERSION: 1.9

Based on: Common Command Input Language - Version: 1996-06-17
ASPEN-DECHEMA Neutral-File-Proposal 1995-12-21

Version: 1.9

Date: 27 September 2011

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Changes & Additions:

Release 1.9:

- Added VIR2 and D104 as new functions

Release 1.8:

- Added STATE as valid keyword for pure component data tables and functions
- Added SAT as new keyword for STATE to indicate saturation (to be used in case of pure component data)
- Added DENC as new unary constant
- Added RINAD, PTCOW, SOLW as new pure component properties

Release 1.7:

- Added DIEC as new pure component property (dielectric constant)
- Added HENRY-P, HENRY-F and PVL as new mixture properties (Henry coefficient with constant partial pressure, Henry coefficient with constant fugacity, partial pressure of a component). The properties are mainly used for GLE data sets.

Release 1.6:

- Added support for private METHODS within the PRIVATE block
- New states: GLE, NO_AZEO, INFIN
- New mixture properties: VE and SE

Release 1.5:

- New keyword VERSION
- New block PRIVATE
- The SYSTEM block is no longer a bracket for SOURCE, COMP-DEF, PURE-COMP-DATA, MIXTURE-DATA and GROUP-PARAMETER. The mentioned blocks can stand for their own on the first level
- Added keyword PHASE for pure component tables and functions
- Rebuild of pure component property list. The combined property-phase identifier like e.g. DENS are dropped (now use PROPERTY DEN plus PHASE S instead)

Editing Rules:

- Lines have less or equal 80 Characters
- Standard ASCII character set (No Umlaut)
- Continuation Sign "&" in column 1
- Comment Sign "!" in column 1 or at any other column to ignore rest of line
- Field Separator "blank" or "tab" (Tabulator)
- For keywords and names the first 12 characters are significant for keyword recognition.
- Keywords case insensitive (title, Title and tTIE are identical keywords)
- Names case sensitive (K2R and k2r are different stream-names)
- Text can be included in "quotes". No quotes are allowed in Text
- Text must be included in "quotes", if the special characters " " (blank), "&" or "!" are used in the text
- Parameters not available are represented by "\$"

- "\$" signs at an end of a line can be omitted.
- There is only 1 statement allowed on a line
- All lines start with a defined keyword or blockname
- Set-ids are used for the connection between THERMODYNAMIC and different models. If a set-id of a model is omitted this version serves as basic version. If parameters of a requested set-id are not found, the basic version parameters are used. Any text string can be used as set-id, e.g. "Set1", "2", "Set Three", "Great Set No. 4", ...
- Standard file extension should be IKC

General Remarks

Units

- Units are text! If blanks are used in units, the unit has to be enclosed in "", e.g. "Pa * s".
- Units are case sensitive. Blanks in unit strings have no meaning and will be ignored.
- A hyphen "-" is used as unit for dimensionless properties.
- Units are processed mathematically. That means you can write e.g. "kg/m^3", "1/(kg^-1*m^3)" or "(m^3/kg)^-1" - all texts mean the same. Remember that "*" following a division sign "/" do not imply, that the following text is part of the division: "kg/m*s^2" is equal to "(kg*s^2)/m". Use e.g. brackets to write "kg/(m*s^2)".
- For convenience "***" can be used instead of "^" for exponents: "m/s^2" is equivalent to "m/s**2".
- Prefixes can be written in front of units, e.g. "mK" means "milli Kelvin". For a list of prefixes see p. 12

Thermodynamic

- The IK-CAPE thermodynamic package is **standard** for all methods and equations. Look up the definitions of methods, equations and parameters in the IK-CAPE thermodynamic package documentation.
- Several thermodynamic blocks with different labels can be defined in the file.

Systems

- Systems are used to group components together with information on thermodynamic and chemical reactions. Different system blocks can be used to describe different units of a process.

Reactions

- The IK-CAPE thermodynamic package is **standard** for all methods and equations. Look up the definitions of equilibrium functions and temperature function in the IK-CAPE thermodynamic package documentation.

Major Keywords ==> Block IDs

VERSION

PRIVATE
END PRIVATE

QUALITY
END QUALITY

SOURCE
END SOURCE

COMP-DEF
END COMP-DEF

PURE-COMP-DA
END PURE-COMP-DA

MIXTURE-DATA
END MIXTURE-DATA

GROUP-METHODS
END GROUP-METHODS

THERMODYNAMIC t_label
END THERMODYNAMIC t_label

CHEM-REAC cr_label
END CHEM-REAC cr_label

SYSTEM s_label
END SYSTEM s_label

Detailed Description

! Optional keywords in a block are marked with an ending * in the following descriptions. Optional keywords
! can be missing in a block, all others must occur in a block. The order of appearance for keywords is free with
! one exception: PROPERTY must occur before any PHASE, UNIT, ERR-UNIT, ERROR, DATA, BOUNDS
! and COEFFICIENTS statement, because the number of items in the PROPERTY sentence is used for error
! checking the number of items in the following sentences.

VERSION "General format" "Release"

! This first sentence is used to identify the Release version used in the file. It will enable parsers to deal with
! files written in different (future) versions of this definition. For this release it must be IKC-PPDX 1.5.

END BLOCKNAME LABELNAME

! End of a Block of Keywords with blockname "BLOCKNAME" and label "LABELNAME" (End may be
! sufficient, but for rigorous error checking this strong syntax is preferred).

PRIVATE*

! Blocks, keywords or methods introduced in the PRIVATE BLOCK will not lead to errors when occurring in file.
! The parser programs will check each line for beginning with a defined keyword or blockname. If the keyword
! or blockname is not defined inside the parser program it can only be a private one not supported by the
! parser or an error.

BLOCKS*	blockid1	blockid2	blockid3
KEYWORDS*	keyword1	keyword2	keyword3
METHODS*	method1	method2	method3

! Private blocks can occur everywhere in the predefined structure. Lines in a private block
! called e.g. "blockid1" are totally ignored by the parser until the "END blockid1" statement occurs (except the
! parser has built-in support for that special, nonstandard block).

! Private keywords can occur everywhere in predefined blocks. Lines in a common block starting with an private
! keyword are totally ignored by the parser (except the parser has built-in support for that special, nonstandard
! keyword).

! Private methods defines valid methods, that are not part of the standard IK-CAPE-PPDX vocabulary (e.g. for
! structures, temperature dependent functions, VLE-equilibrium etc.) BLOCKS or STATEMENTS for such a
! private method will have the same syntax and contents as a standard (predefined) block and should be processed
! by standard parsers without errors or warnings. Standard parsers even should be able to write such a block.

END PRIVATE

QUALITY*

QKEY quality-key "Explanation"

! Defines a quality-key and gives some explanation about it
! All quality-keys used in the following must be defined here. If not, a warning is given.

END QUALITY

SOURCE*

! Description of a Data-Source ==> Reference

KEY	source-key		! The source-key is used for referencing in the following
AUTHOR*	"author"		! Author of reference
TITLE*	"title"		! Title of reference
JOURNAL*	"journal"		! Journal name of reference
CODEN*	"coden"		! Unique key (originated from Chemical Abstracts)
VOLUME*	"volume"		! Volume number usually indicates publication year
ISSUE*	"issue"		! Issue number usually indicates publication month
PAGE*	"page"		! Page where reference can be found
YEAR*	"year"		! Publication year
ISBN*	"isbn"		! International standard book number

ISSN* "issn" ! International standard serial number (The ISBN for periodicals)
END KEY source-key

END SOURCE

COMP-DEF

! Define components by component id (cid) and additional data

CID cid ! The cid is referenced in the following
NAME* "name"
SYNONYM* "synonym"
CAS-NO* "CAS-No"
FORMULA* "formula" ! Hill format
STRUCTURE* method grpid1 n1 ! see list on p. 11
& grpid2 n2 grpid3 n3 grpid4 n4
! If an unknown method name is used in a STRUCTURE sentence a
! warning message is given, but the parser has to process the
! sentence.
END CID cid

END COMP-DEF

PURE-COMP-DA*

! Enter Data for pure components

PROPERTIES*

Property set-id cid value unit err-value err-unit quality-key source-key
! for a list of valid properties see p. 8

END PROPERTIES

! End of pure component properties

PARAMETERS*

Method parameter set-id cid value unit quality-key source-key
! for a list of valid methods and parameters see p. 10

END PARAMETERS

TABLE* label set-id

COMPONENT cid
SOURCE-KEY* source-key
QUALITY* quality-key
STATE state-key ! for a list of valid states see p. 7
! STATE can be omitted, if not necessary
PROPERTY prop1 prop2 prop3 ... ! for a list of properties see p. 8
PHASE* phase1 phase2 phase3 ... ! for a list of phases see p. 7
! PHASE can be omitted, if not necessary for property recognition
UNIT unit1 unit2 unit3 ...
ERR-UNIT* errunit1 errunit2 errunit3 ...
! when ERR-UNIT is omitted ERROR is of same unit as DATA
ERROR* errval1 errval2 errval3 ...
! Error data valid till next ERROR statement
DATA value1 value2 value3 ...

...

END TABLE label

FUNCTION* label set-id

NAME function-name ! for a list of names see p. 11
COMPONENT cid
SOURCE-KEY* source-key
QUALITY* quality-key
STATE state-key ! for a list of valid states see p. 7
! STATE can be omitted, if not necessary
PROPERTY y-prop xprop1 xprop2 ...
PHASE* y-phase xphase1 xphase2 ... ! for a list of phases see p. 7
! PHASE can be omitted, if not necessary for property recognition
UNIT y-unit x-unit1 x-unit2 ...

BASIC* b_label ! This label gives the basic thermodynamic block for ! t_label. Omitted information is filled from the block ! b_label.

PROPERTIES* ! Properties to be used in this thermodynamic block.
property set-id ! For a list of valid properties see p. 8. If a property is
END PROPERTIES ! omitted, the basic version is used.

PARAMETERS* ! Parameters to be used in this thermodynamic block.
method parameter set-id ! For a list of valid methods and parameters see p. 10
END PARAMETERS ! If a parameter is omitted, the basic version is used.

PURE* ! Methods for pure component property calculation
property function-name set-id ! For list of properties see p. 8, for list of function-names
END PURE ! see p. 11

VLEQ* ! Methods for VLEQ calculation.
ACTIVITY* method set-id ! Method for γ calculation. IDEAL, if not defined.
FUGACITY* method set-id ! Method for ϕ calculation. IDEAL, if not defined.
POYNTING* boolean ! Usage of Poynting correction: TRUE or FALSE.
HENRY* boolean set-id ! Usage of Henry for inerts: TRUE or FALSE. If TRUE,
! all components with METHOD HENRY VLE set-id
! definitions are used as inerts in calculation.
EOS* method set-id ! Default value for POYNTING and HENRY is FALSE.
! usage of method for ϕ - ϕ calculation. Overwrites
! all ACTIVITY, FUGACITY, POYNTING and HENRY
! statements, if given.

END VLEQ

LLEQ* ! If LLEQ is not defined, the VLEQ ACTIVITY
ACTIVITY method set-id ! method is used.
END LLEQ

ENTHALPY* ! Methods for enthalpy calculation
ACTIVITY method set-id ! Method for h_e calculation
PRESS-CORR method set-id ! Method for dp calculation
STARTPHASE cid phase ! Reference phase for starting enthalpy calculation
TREF cid tref unit ! Temperature for starting point of calculation
HREF cid href unit ! Enthalpy for starting point of calculation
T-PH-CH cid t-ph-ch unit ! Temperature for calculation of phase change
END ENTHALPY

ENTROPY* ! Methods for entropy calculation
ACTIVITY method set-id ! Method for s_e calculation
PRESS-CORR method set-id ! Method for ϕ calculation
STARTPHASE cid phase ! Reference phase for starting entropy calculation
TREF cid tref unit ! Temperature for starting point of calculation
SREF cid href unit ! Entropy for starting point of calculation
T-PH-CH cid t-ph-ch unit ! Temperature for calculation of phase change
END ENTROPY

MIXCALC* ! Methods for calculation of averages in mixtures.
property* phase method ! For list of properties see p. 9, for average methods p. 11.
property* phase method set-id ! In addition (especially for vapor phase density) also the
END MIXCALC ! methods given on p. 12 can be used.

END THERMODYNAMIC t_label

CHEM-REAC* cr_label ! For a list of reaction types see p. 12

RATE* Reac-Nr.
HREAC value unit
STOIC cid1 coeff1 cid2 coeff2 ... ! stoichiometric coefficients: positive values for
! coefficient are products, negative values are educts

RATE value ! unit ist kmol/s
 END RATE Reac-Nr.

CONVERSION* Reac-Nr.
 HREAC value unit
 STOIC cid1 coeff1 cid2 coeff2 ...
 CONVERSION Conversion cid ! cid must occur in STOIC with negative coefficient
 END CONVERSION Reac-Nr.

STATE* Reac-Nr.
 HREAC value unit
 STOIC cid1 coeff1 cid2 coeff2 ...!
 CONVERSION Conversion cid ! cid must occur in STOIC with negative coefficient
 END STATE Reac-Nr.

EQUIL* Reac-Nr.
 TYPE Type ! for a list of Equilibrium types see p. 12
 HREAC value unit
 STOIC cid1 coeff1 cid2 coeff2 ...
 F(T) a b c d e f unit ! six coefficients for Equilibrium function
 END EQUIL Reac-Nr.

KINETIC* Reac-Nr.
 TYPE Type ! for a list of Kinetic reaction types see p. 12
 HREAC value unit
 STOIC cid1 coeff1 cid2 coeff2 ...
 F(T) F-Label a b c d unit ! four coefficients for temperature function
 ALPHA F-Label Cid1 value Cid2 value ... ! coefficients for corresponding concentration function
 ! The F-Label gives the correspondence between ALPHA and F(T)
 PHI(T) P-Label a b c d unit ! four coefficients for temperature function (catalyst)
 GAMMA P-Label Cid1 value Cid2 value ... ! coefficients for corresponding concentration function
 ! The P-Label gives the correspondence between GAMMA and PHI(T)
 END KINETIC Reac-Nr.

END CHEM-REAC cr_label

SYSTEM* s_label ! Different SYSTEM blocks can be used to describe
 COMPONENTS cid1 cid2 cid3 ... ! various units in a process. The system blocks defines
 THERMODYNAMIC t_label ! the components present in the unit, the thermodynamic
 CHEM-REAC* cr_label ! to be used for calculation and (if necessary) the
 END SYSTEM s_label ! chemical reaction taking place.

List of general usage properties

T Temperature
 P Pressure
 X Component fraction in liquid phase ! Phase can be: L, L1, L2, ...
 ! first X refers to first cid, second to second cid, ...
 Y Component fraction in vapor phase ! Phase can be: V
 ! first Y refers to first cid, second to second cid, ...
 S Component fraction in solid phase ! Phase can be: S, S1, S2, ...
 ! first S refers to first cid, second to second cid, ...

List of Phases

L Liquid phase
 L1, L2, ... Liquid phase 1, liquid phase 2, ...
 V Vapor phase
 S Solid phase
 S1, S2, ... Solid phase 1, solid phase 2, ...

List of State Flags

SAT Saturation (to be used in case of pure component data)

VLE	Vapor-Liquid-Equilibrium
LLE	Liquid-Liquid-Equilibrium
VLLE	Vapor-Liquid-Liquid-Equilibrium
SLE	Solid-Liquid-Equilibrium
GLE	Gas-Liquid-Equilibrium
CHEM-EQ	Chemical Equilibrium
AZEO	Azeotrop
NO_AZEO	Not an Azeotrop
INFIN	At infinite solution

List of Properties (Pure Component Constant Properties)

MW	Molecular Weight
TC	Critical Temperature
PC	Critical Pressure
VC	Critical Volume
DENC	Critical Density
ZC	Critical Compressibility Factor
OMEGA	Acentric Factor
TB	Normal boiling point (1 atm)
TMP	Normal melting point (1 atm)
HLVB	Heat of vaporization at normal boiling point
HLSM	Heat of melting at normal melting point
HF0V	Standard Heat of formation (Vapor)
HF0L	Standard Heat of formation (Liquid)
HF0S	Standard Heat of formation (Solid)
GF0V	Standard Free energy of formation (Vapor)
GF0L	Standard Free energy of formation (Liquid)
GF0S	Standard Free energy of formation (Solid)
SOV	Standard Entropy (Vapor)
SOL	Standard Entropy (Liquid)
SOS	Standard Entropy (Solid)
PARA	Parachor
DIPM	Dipole moment
RGYR	Radius of gyration (in german: Trägheitsradius)
VOL0	Volume at standard conditions

"0" in property names characterizes standard conditions

Standard is at 25 °C and 1 atmosphere, vapor refers to ideal gas phase

List Pure Component Properties (T and/or P dependent)

PVL	Vapor pressure	
PSV	Sublimation pressure	
PSL	Melting pressure	
HLV	Heat of vaporization	
HSV	Heat of sublimation	
HSL	Heat of melting	
CPIG	Heat Capacity of ideal gas	
CP	Heat Capacity	! Phase sentence necessary
DEN	Density	! Phase sentence necessary
DIEC	Dielectric constant	
VOL	Specific volume	! Phase sentence necessary
VIS	Viscosity	! Phase sentence necessary
K	Thermal conductivity	! Phase sentence necessary
SFTN	Surface tension	
VIR2	Second virial coefficient	
VIR3	Third virial coefficient	
H	Enthalpy	! Phase sentence necessary
S	Entropy	! Phase sentence necessary
G	Gibbs energy	! Phase sentence necessary
HF	Heat of formation	! Phase sentence necessary
GF	Gibbs energy of formation	! Phase sentence necessary
RINAD	Refractive Index, Na-D-Line	

List of Mixture Properties

TBUB	Bubble Point	
TDEW	Dew Point	
PBUB	Pressure at Bubblepoint	
PDEW	Pressure at Dewpoint	
DEN	Density	
VOL	Volume	
VIS	Viscosity	
K	Thermal Conductivity	
SFTN	Surface Tension	
HE	Excess Enthalpy	
GE	Excess Gibbs Energy	
CPE	Excess Heat capacity	
VE	Excess Volume	
SE	Excess Entropy	
H	Enthalpy	
G	Gibbs Energy	
S	Entropy	
CP	Heat Capacity	
ACTI	Activity Coefficient	
FUGA	Fugacity Coefficients	
ACTI+	Activity Coefficient for Anions in electrolyte data	
ACTI-	Activity Coefficient for Kations in electrolyte data	
OSMO	Osmotic Coefficient	! first coefficient refers to first cid, second to second cid, ...
BUNSEN	Bunsen Coefficient	! first coefficient refers to first cid, second to second cid, ...
OSTWALD	Ostwald Coefficient	! first coefficient refers to first cid, second to second cid, ...
KUENEN	Kuenen coefficient	! first coefficient refers to first cid, second to second cid, ...
HENRY	Henry coefficient	! first coefficient refers to first cid, second to second cid, ...
HENRY-P	Henry coefficient (partial pressure)	! first coefficient refers to first cid, second to second cid, ...
HENRY-F	Henry coefficient (Fugacity)	! first coefficient refers to first cid, second to second cid, ...
PVL	Partial pressure	! first coefficient refers to first cid, second to second cid, ...

List of Binary Property Methods & Matrices

! Method	Matrix	
NRTL	ALPHA	! NRTL method for γ calculation
NRTL	BETA	
NRTL	A	
NRTL	B	
NRTL	C	
NRTL	D	
WILSON	A	! Wilson method for γ calculation
WILSON	B	
WILSON	C	
WILSON	D	
UNIQUAC	B	! UNIQUAC method for γ calculation
MODUNIQUACA		! Modified UNIQUAC method for γ calculation
MODUNIQUACB		
MODUNIQUACC		
MODUNIQUACD		
HENRY	A	! Henry method for inerts in VLEQ calculation
HENRY	B	
HENRY	C	
HENRY	D	
RKS	K	! Redlich-Kwong-Soave method for ϕ calculation

PR	K	! Peng-Robinson method for ϕ calculation
DIFV	D	! Diffusion-coefficients of gases
DIFL	D	! Diffusion-coefficients of liquids

List of Property Methods & Parameters

! Method name	Parameter1, Parameter2, ...	
UNIQUAC	R, Q	! UNIQUAC parameters
MODUNIQUAC	R, Q, Q'	! Modified UNIQUAC parameters
RKS	A, B	! Redlich-Kwong-Soave parameters
PR	A, B	! Peng-Robinson parameters
FLORY-HUGGIN	R, CHI0, CHI1	! Flory-Huggins parameters
DMER	A, B	! Dimerisation parameters
TMER	A, B	! Tetramerisation parameters
HMER	A, B	! Hexamerisation parameters

List of Group-Methods for Keyword STRUCTURE

! Group method	Matrix sign	
LYDERSEN	M	! Lydersen
JOBACK	M	! Joback
UNIFAC	B	! Standard UNIFAC-Method
D-UNIFAC	B, C, D	! Modified UNIFAC Dortmund
L-UNIFAC	B, C, D	! Modified UNIFAC Lyngby

List of Functions to describe Temperature Dependencies

POLYNOM	! Polynom
EPOLYNOM	! Exponential Polynom
ANTOINE	! Antoine
EXANTOINE	! Extended Antoine
WATSON	! Watson
WAGNER	! Wagner
SUTHERLAND	! Sutherland
KIRCHHOFF	! Kirchhoff
RACKETT	! Rackett
CPL1	! Heat Capacity of Liquids (HOECHST CPL)
CPL2	! Heat Capacity of Liquids (HOECHST ICPL)
VIS1	! Viscosity of Liquids (HOECHST VISC)
ALYLEE	! Aly-Lee
KIR1	! Modified Kirchhoff (DIPPR)
DIP4	! DIPPR equation for heat of vaporization and surface tension
DIP5	! DIPPR equation for thermal conductivity and viscosity of gases
VIR2	! Model for second virial coefficient
D104	! DIPPR 104 model for second virial coefficient

List of Average Methods

MOLA	! Average on molar basis
MASS	! Average on mass basis
MOL-LOG	! Average on logarithmic molar basis
MASS-LOG	! Average on logarithmic mass basis
VOLU	! Average on volumetric basis
KVAP	! Special for thermal conductivity of gases
VISV	! Special for viscosity of gases
WILK	! Wilke method for viscosity of gases
WAMA	! Wassilijewa, Mason, Saxena method for thermal conductivity of gases
DIST	! Average for surface tension from DIPPR
DIKL	! Average for liquid thermal conductivity from DIPPR

List of Functions for Extrapolation

LINEAR	! Linear extrapolation
FIXED-BOUND	! Function converges to bound "value"
EXPONENTIAL	! Linear extrapolation in a logarithmic diagram
WAGNER	! Special extrapolation of Wagner equation

List of Methods for Vapor-Liquid Activity-Coefficients

IDEAL
NRTL
UNIQUAC
MODUNIQUAC
WILSON
FLORY-HUGGIN
UNIFAC
D-UNIFAC
L-UNIFAC

List of Methods for Liquid-Liquid Activity-Coefficients

NRTL
UNIQUAC
MODUNIQUAC
UNIFAC
D-UNIFAC
L-UNIFAC

List of Methods for Vapor Phase Mixture Calculations

IDEAL
PR
RKS
PMER
VIRI

List of Reaction types

CONVERSION	conversion reaction based on total incoming flows to the unit
STATE	conversion reaction based on the state of the system, taking into account all chemical reactions and possible phase changes
COORDINATE	given reaction rate
EQLM	Equilibrium reaction based on liquid mole fraction
EQVM	Equilibrium reaction based on vapor mole fraction
EQLC	Equilibrium reaction based on liquid concentration
EQVC	Equilibrium reaction based on vapor concentration
EQLA	Equilibrium reaction based on liquid activity
EQVP	Equilibrium reaction based on partial pressure
EQLF	Equilibrium reaction in the liquid phase based on fugacity
EQVF	Equilibrium reaction in the vapor phase based on fugacity
KILM	Kinetic reaction based on liquid mole fraction
KILC	Kinetic reaction based on liquid concentration
KIVM	Kinetic reaction based on vapor mole fraction
KIVC	Kinetic reaction based on vapor concentration
KILW	Kinetic reaction based on liquid mass fraction
KIVW	Kinetic reaction based on vapor mass fraction

List of Prefixes for Units

! Prefix	Meaning	Name
E	1.0E+18	Exa
P	1.0E+15	Peta
T	1.0E+12	Tera
G	1.0E+9	Giga
M	1.0E+6	Mega
k	1.0E+3	Kilo
h	1.0E+2	Hekto
da	1.0E+1	Deka
a	1.0E-18	Atto
f	1.0E-15	Femto
p	1.0E-12	Pico
n	1.0E-9	Nano
u	1.0E-6	Mikro
m	1.0E-3	Milli
c	1.0E-2	Zenti
d	1.0E-1	Dezi

EXAMPLE for an IK-CAPE-PPDX file

```
!  
! Remember: The data given in this example are absolutely nonsense!  
!  
VERSION      IKC-PPDX      1.7  
  
PRIVATE  
  KEYWORDS   PRIV_KEY_1  
  BLOCKS     PRIV_BLOCK_1 PRIV_BLOCK_2  
  METHODS    MY_METHOD1  
END PRIVATE  
  
QUALITY  
  QKEY      1      "very good"  
  QKEY      2      "good"  
  QKEY      3      "average"  
  QKEY      4      "bad"  
END QUALITY  
  
SOURCE  
  KEY Ref-1  
    AUTHOR   "Author, A.B.; Author, C.D."  
    TITLE    "The title of this 'ole' document"  
    JOURNAL  "A Journal"  
    CODEN    JCEAAX  
    VOLUME   32  
    ISSUE    4  
    PAGE     420-422  
    YEAR     1987  
    ISSN     123456789  
    PRIV_KEY_1 "Mr. Meyer, Office 7.2, 7th floor"  
    ! Who owns this document as sample for private keyword usage  
  END KEY Ref-1  
END SOURCE  
  
COMP-DEF  
  CID      MeOH  
    NAME    Methanol  
    FORMULA CH4O  
    SYNONYM Holzgeist  
    CAS-NO  65-12-03  
    STRUCTURE JOBACK      CH3 1 OH 1  
  END CID MeOH  
  CID      H2O  
    NAME    Water  
    FORMULA H2O  
    SYNONYM Wasser  
  END CID H2O  
  CID      C6H6  
    NAME    Benzene  
    FORMULA C6H6  
  END CID C6H6  
  CID      CO2  
    NAME    Carbon dioxide  
    FORMULA CO2  
  END CID CO2  
END COMP-DEF
```

PURE-COMP-DATA

PROPERTIES

MW	\$	MeOH	36.5	kg/kmol	\$	\$	2	Ref-1
TB	\$	MeOH	64.8	C	\$	\$	2	Ref-1

END PROPERTIES

PARAMETERS

UNIQUAC	r	\$	MeOH	3.5
UNIQUAC	q	\$	MeOH	4.1
UNIQUAC	r	1	MeOH	3.84
UNIQUAC	q	1	MeOH	4.67

END PARAMETERS

TABLE vap-press

COMPONENT	MeOH
SOURCE-KEY	Ref-1
PROPERTY	PVL T
UNIT	mbar C
ERROR	5 1
DATA	120 10.
DATA	180. 20.
DATA	220 30.
ERROR	8. 2
DATA	300. 50.
DATA	1000. 4.8

END TABLE vap-pres

FUNCTION vap-pres

NAME	ANTOINE
COMPONENT	MeOH
QUALITY	2
PROPERTY	PVL T
UNIT	Torr C
LOWER-BOUND	0.
UPPER-BOUND	150.
COEFFICIENTS	123. -34. 250.

END FUNCTION vap-pres

PRIV_BLOCK_1

...

...

END PRIV_BLOCK_1

END PURE-COMP-DATA

MIXTURE-DATA

TABLE h

COMPONENTS	MeOH	H2O
PROPERTY	T	X H
PHASE	L	L L
UNIT	C	mol/mol kJ/kg
DATA	10.	.5 2350.
DATA	20.	.5 2360.
DATA	10.	.6 2420.
DATA	20.	.6 2425.

END TABLE h

TABLE vle

COMPONENTS	MeOH	H2O
STATE	VLE	
PROPERTY	T	P X Y
UNIT	C	bar mol/mol mol/mol
DATA	60.	1.1 .5 .3

DATA 80. 1.1 .4 .2
END TABLE vle

TABLE lle

COMPONENTS	H2O	MeOH	C6H6		
PROPERTY	T	X	X	X	X
PHASE	\$	L1	L2	L1	L2
UNIT	K	mol/mol	mol/mol	mol/mol	mol/mol
DATA	299.15	0.95886	0.00516	0.04067	0.00798
DATA	299.15	0.83843	0.00807	0.16052	0.02389
DATA	299.15	0.63984	0.01051	0.35282	0.03783
DATA	299.15	\$	0.8383	\$	0.1605
DATA	299.15	\$	0.7249	\$	0.2715
DATA	299.15	0.1218	\$	0.4982	\$
DATA	299.15	0.1102	\$	0.4541	\$

END TABLE lle

TABLE gle

COMPONENTS	CO2	H2O		
PROPERTY	T	HENRY-P		PVL
UNIT	C	Pa*mol/mol		Pa
DATA	60.	1E+8		1.1013
DATA	80.	1.3E+8		1.1013

END TABLE vle

BINARY-PARAM

METHOD NRTL VLE Set-1

Alpha	MeOH	H2O	0.2	0.2
A	MeOH	H2O	3.5	4.3
B	MeOH	H2O	2.1	3.2

END METHOD NRTL

METHOD PR VLE Set-1

K	MeOH	H2O	0.12	0.12
K	MeOH	C6H6	0.02	0.02
K	H2O	C6H6	0.21	0.21

END METHOD PR

METHOD PR VLE Set-EOS

K	MeOH	H2O	0.11	0.11
K	MeOH	C6H6	0.82	0.82
K	H2O	C6H6	0.23	0.23

END METHOD PR

METHOD MY_METHOD1 VLE Set-1

A	MeOH	H2O	1.23	2.34
B	MeOH	H2O	4.56	6.78

END METHOD MY_METHOD1

METHOD NRTL LLE Set-1

Alpha	MeOH	H2O	0.3	0.3
A	MeOH	H2O	1.1	2.2
BOUNDS-T	0	100	C	
BOUNDS-X	0	0.2	mol/mol L1	MeOH
BOUNDS-X	0.9	1.0	mol/mol L2	MeOH

END METHOD NRTL

END BINARY-PARAM

PRIV_BLOCK_2

...
...

END PRIV_BLOCK_2

END MIXTURE-DATA

GROUP-METHODS

```

G-PARAMETER
  METHOD D-UNIF      r      q
      CH3   1      2.5    3.8
      OH    5      1.2    2.7
  END METHOD D-UNIF
END G-PARAMETER

```

```

G-INTERACTION
  METHOD D-UNIF
      B     1     3     1.1   2.3
      B     1     5     2.0   1.1
      B     5     7     2.3   2.2
  END METHOD D-UNIF
END G-INTERACTION

```

END GROUP-METHODS

THERMODYNAMIC T1

```

VLEQ
  ACTIVITY  NRTL  Set-1
  FUGACITY  PR    Set-1
  POYNTING  TRUE
END VLEQ

```

```

LLEQ
  ACTIVITY  NRTL  Set-1
END LLEQ

```

ENTHALPY

```

  ACTIVITY  NRTL  Set-1
  PRESS-CORR PR    Set-1
  STARTPHASE MeOH  L
  STARTPHASE H2O   L
  STARTPHASE C6H6  V
  TREF      H2O   298.15 K
  TREF      MeOH  298.15 K
  TREF      C6H6  298.15 K
  HREF      H2O   23.000 J/mol
  HREF      MeOH  12.230 J/mol
  HREF      C6H6  45.560 J/mol
  T-PH-CH   H2O   340    K
  T-PH-CH   MeOH  340    K
  T-PH-CH   C6H6  323.15 K
END ENTHALPY

```

MIXCALC ! The functions for the different components are not given in this example, assume they are

```

...
  VIS  L    MOLA
  DENS V    PR    Set-1

```

END MIXCALC

END THERMODYNAMIC T1

THERMODYNAMIC T2

```

  BASIC T1
  VLEQ
      EOS      PR    SET-EOS
  END VLEQ

```

END THERMODYNAMIC T2

SYSTEM S1
COMPONENTS MeOH H2O
THERMODYNAMIC T1
END SYSTEM S1

SYSTEM S2
COMPONENTS MeOH H2O C6H6
THERMODYNAMIC T2
END SYSTEM S2