
Korean Thermophysical Properties DataBank

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물성 데이터베이스의 필요성

- 화학공학 산업의 다각화 및 신기술의 등장으로 인한 물성 및 상평형 자료의 필요성
- 공정모사기, 공정설계 프로그램들의 바탕을 이루는 열역학 Databank 및 계산모듈의 국산화 필요
- 외국 물성 Databank 의 고가 서비스로 인한 비용 증가

해외관련 기술 현황-DETERM(독일)

- 개발기관 : DECHEMA/Dortmund University
- 평형자료 DB 로서는 세계 최고 규모
- 제공 data base
 - ◆ Reference : 약 14,000개
 - ◆ 순수성분 물성치 : 약 7,000 성분
 - ◆ 상평형 데이터, 과잉 엔탈피 등 : 약 620,000 개
- 제공 유형
 - ◆ On-line access, In-house version, Internet access

해외관련 기술 현황-DETERM(독일)

- Contents of DETERM

Package Name	No. of Data Points	Contents
DDB	245,000	VLE,LLE,HE,CPE, Pure properties
ELDAR (Electrolyte)	50,622	Density, Heat of solutions, heat capacities, viscosity
INFOTHERM	71,272	PVT data, Surface, caloric and equilibrium(VLE,LLE,GLE) data
COMDOR	20,131	VLE equilibria, Excess enthalpy
C-DATA	7,047	20 physico-chemical properties of 539 chemicals
BDBB	18,041	Properties constant matrix with 25 fields for 1126 components
OTHERS	208,627	Chebychev- and Antoine constants, transport properties, critical constants

해외관련 기술 현황-DIPPR(미국)

- 1980년대 초 미국 AIChE 주관 Penn. State University 등에서 시작
- 탄화수소류 위주의 data compilation
 - ◆ 기존 문헌의 실험 자료 수집
 - ◆ 실험자료의 평가 및 상관식, 예측식의 개발
 - ◆ 실험을 통한 data matrix의 완성
- 현재 1735 종의 성분에 대한 자료 확보
 - ◆ 29개의 고정물성과 15개의 온도 의존 물성 포함
- 연간 예산 약 500,000 \$

Korean Thermophysical Properties DataBank (KDB)

- 1996년 통상산업부(현 산업자원부) 지원하에 과제 수행 (1996-98년, 3년간)
- 고려대학교, 서강대학교, 서울대학교, KAIST 참여
- 1998년 이후 고려대학교 화공정보센터의 지원하에 관리 및 유지

KDB 개발방향

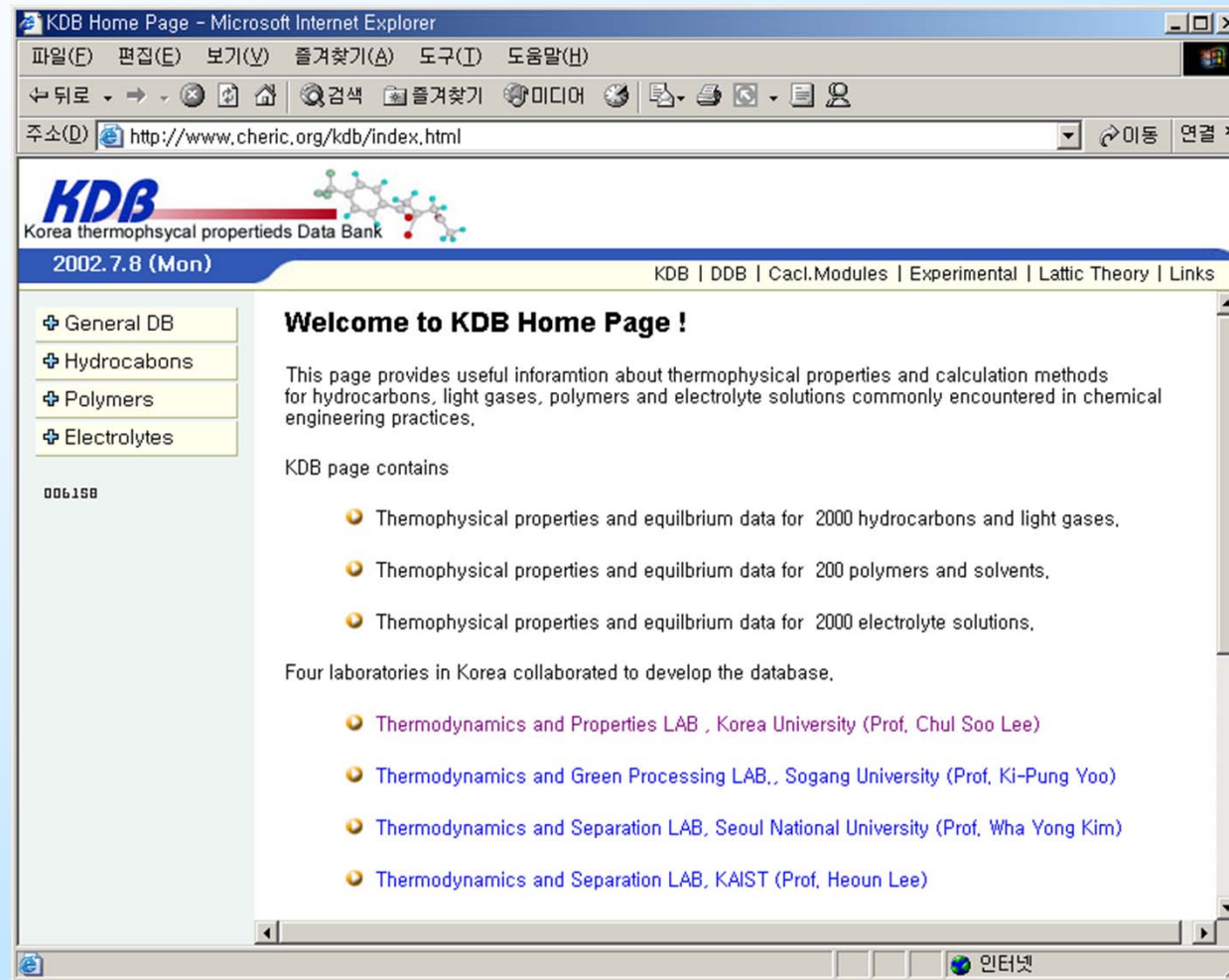
- 자료 입력 및 축적
- 자료관리 시스템 개발
- 물성, 상평형 계산 프로그램 및 인터페이스 개발
- 물성 및 상평형 계산 모델의 평가

KDB 개발 체계

- 고려대학교 화공생명공학과 열역학 및 물성연구실
 - ◆ 탄화수소류, 전해질, 고분자계의 열역학 물성 측정
 - ◆ 열역학 모델 개발
 - ◆ 열역학 물성 계산 프로그램 공급

- 고려대학교 화학공학정보센터
 - ◆ Database 관리
 - ◆ 인터넷 서비스

KDB WEB Home Page



KDB general databank

- 원자량

KDB Home Page - Microsoft Internet Explorer

http://www.cheic.org/kdb/index.html

KDB Korea thermophysical properties Data Bank

2002. 7. 17 (Wed)

KDB | DBB | Cacl.Modules | Experimental | Latic Theory | Links

General DB

- Atomic Weights
- Units
- Constants
- Hydrocabons
- Polymers
- Electrolytes

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Periodic Table of Elements

Atomic weights shown in this table are 1977 values.
For long-lived isotope of an element that has no stable isotopes, standard atomic weights cannot be defined because of wide variety of isotopic composition in nature.
For these elements, refer to "Atomic masses and abundances" table in the following references.

- D.R.Linde ed., "CRC handbook of Chemistry and Physics", 76th ed., CRC Press, Boca Raton (1995)
- IUPAC Commission on Atomic Weights and Isotopic Abundances, Pure Appl. Chem., 63, 991 (1991)

Atom No.	Group	Name	Symbol	Atom.Wt. (g/mol)
1	1A	Hydrogen	H	1.0079
2	0	Helium	He	4.0026
3	1A	Lithium	Li	6.941
4	2A	Beryllium	Be	9.01218
5	3A	Boron	B	10.81
6	4A	Carbon	C	12.011
7	5A	Nitrogen	N	14.0067
8	6A	Oxygen	O	15.9994
9	7A	Fluorine	F	18.9984
10	0	Neon	Ne	20.179
11	1A	Sodium	Na	22.98977
12	2A	Magnesium	Mg	24.305
13	3A	Aluminium	Al	26.98154
14	4A	Silicon	Si	28.0855
15	5A	Phosphorus	P	30.97376
16	6A	Sulfur	S	32.06
17	7A	Chlorine	Cl	35.453
18	0	Argon	Ar	39.948
19	1A	Potassium	K	39.0983

KDB general databank

- Units

KDB
Korea thermophysical properties Data Bank

2002. 7. 17 (Wed)

General DB
Atomic Weights
Units
Constants
Hydrocarbons
Polymers
Electrolytes

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KDB
Korea thermophysical properties Data Bank

2002. 7. 17 (Wed)

KDB | DDB | Calc.Modules | Experimental | Lattice Theory | Links

Unit Conversion

[Instruction]

- Select unit you convert (1).
- Enter value you wish to convert (2).
- If you want conversion between molar and weight based units, enter molecular weight (3).
- Press button to convert the value.

(1) Select unit: Pa

(2) Value to convert: 60000

Conversion Back to Unit Selection

Equal values	
=	6.000000E+004 Pa
=	6.000000E+001 kPa
=	6.000000E-002 MPa
=	6.118297E-001 kg/cm ²
=	6.000000E-001 bar
=	5.921540E-001 atm
=	8.70226 psi
=	1.253126E+003 psf
=	6.000000E+005 dyn/cm ²

KDB general databank

- 상수(Constants)

The screenshot shows the KDB Home Page in Microsoft Internet Explorer. The browser window title is "KDB Home Page - Microsoft Internet Explorer". The address bar shows the URL "http://www.therc.org/kdb/index.html". The page content includes the KDB logo and the text "Korea thermophysical properties Data Bank". The date "2002. 7. 17 (Wed)" is displayed. The navigation menu includes "General DB", "Atomic Weights", "Units", "Constants", "Hydrocarbons", "Polymers", and "Electrolytes". The "Constants" section is expanded, showing a list of universal constants with their values in different units.

Constant	Value 1	Value 2
Gas Constants		
	8.314390E+00 J/mol.K	8.314390E+00 Pa.m ³ /mol.K
	8.205670E+01 atm.cm ³ /mol.K	8.205670E-02 atm.l/mol.K
	8.314390E+01 bar.cm ³ /mol.K	1.987190E+00 Btu/lb-mol.R
	1.073000E+01 psi.ft ³ /lb-mol.R	6.236310E+01 mmHg.l/mol.K
	1.987190E+00 cal/mol.K	
Avogadro Number	6.022137E+23 /mol	
Boltzmann's Constant	1.380658E-23 J/K	1.380658E-16 erg/K
	8.617385E-05 eV/K	
Speed of Light	2.997924E+08 m/s	
Element Charge	1.602177E-19 C	
Faraday Constant	9.648531E+04 C/mol	
Plank Constant	6.626076E-34 J.s	1.054573E-34 J.s /2 pi

KDB 순수성분 데이터

- Organics and gases (1941 종)
 - ◆ Freezing point temp., boiling point temp., critical properties, dipole moment and so on (30개).
- Polymers (194 종)
 - ◆ Glass transition temp., melting point, solubility parameter, liquid heat capacity, cohesive energy and so on (24 개)
- Inorganics and Electrolytes (2382 종)
 - ◆ Melting point, heat capacity, entropy of formation, enthalpy of formation and so on (9 개)

KDB 순수성분 물성

KDB Home Page - Microsoft Internet Explorer
주소(D) http://www.theric.org/kdb/index.html

KDB
Korea thermophysical properties Data Bank

2002. 7. 8 (Mon) KDB | DDB | Calc.Modules | Experimental | Lattice Theory | Links

General DB
Hydrocarbons
Pure Properties
Binary VLE
Polymers
Electrolytes

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Pure Component Properties

Search method (1) : Enter search string ...

Component Name	<input type="text" value="methane"/>	ex) methane,...
Component Formula	<input type="text"/>	ex) CH4,H2O...
CA Registry No.	<input type="text"/>	ex) 142-82-5,...

Search

Search method (2) : Select component classification ...

- Paraffinic Hydrocarbons (n-Alkanes)
- Paraffinic Hydrocarbons (Branched Alkanes)
- Unsaturated Hydrocarbons (Alkenes)
- Unsaturated Hydrocarbons (Alkadienes)
- Unsaturated Hydrocarbons (Alkynes)
- Naphthenic Hydrocarbons (Cycloalkanes)
- Naphthenic Hydrocarbons (Unsaturated naphthenes)
- Aromatics (Alkyl Benzene)
- Aromatics (Unsaturated Aromatics)
- Aromatics (Polyaromatics)
- Alcohols (Aliphatic Alcohols)
- Alcohols (Aromatic Alcohols)
- Alcohols (Unsaturated or Cyclic Alcohols)
- Alcohols (Polyols)

KDB 순수성분 물성

The screenshot displays the KDB (Korea thermophysical properties Data Bank) website interface. The main content area is titled "Temperature Dependent Properties" and shows data for Methane (CH₄). A graph plots Vapor Pressure (PVP) in kPa against Temperature in K, showing a non-linear increase. Below the graph, a table provides the KDB Correlation Equation and its coefficients.

Temperature Dependent Properties
 [PVP] Vapor pressure of METHANE

PVP (kPa) of METHANE

Temperature (K)	PVP (kPa)
90	~10
100	~20
110	~40
120	~80
130	~150
140	~300
150	~600
160	~1200
170	~2200
180	~4000
190	~7000

Equation Name	KDB Correlation Equation
Equation	$\ln(P_{vp}) = A + \ln(T) + B/T + C + D \cdot T^2$ where Pvp in kPa, T in K
Coefficient A	-2,374836E+00
Coefficient B	-1,238032E+03
Coefficient C	2,664952E+01
Coefficient D	2,048824E-05
Coefficient E	

KDB 혼합물 평형 데이터

- Organic mixtures
 - ◆ Vapor-liquid equilibria : 4979 sets (68,392 points)
- Polymer systems
 - ◆ Vapor-liquid equilibria : 431 sets (3,037 points)
 - ◆ Infinite activity data : 222 points
- Electrolyte systems
 - ◆ Vapor-liquid equilibria : 502 sets (5,615 points)
 - ◆ Solubility data : 501 sets (9,349 points)

KDB 혼합물 평형 데이터

KDB Korea thermophysical properties Data Bank
2002. 7. 8 (Mon)

Navigation: General DB, Hydrocarbons, Pure Properties, Binary VLE, Polymers, Electrolytes

Search Results:

No.	
1	1914
2	817

Binary Vapor-Liquid Equilibrium Data

Isothermal P-T-X-Y Data : METHANOL + WATER at 323,15K
Reference: Kurihara, K., T. Minoura, K. Takeda and K. Kojima, J. Chem. Eng. Data, 40, 679 (1995)
Method:

Number of Data Points = 14

T, K	P, kPa	X	Y	T Err	P Err	X Err	Y Err
323,15	29,119	0,2470	0,6710	+-0,01	+-0,03		
323,15	30,620	0,2642	0,7029	+-0,01	+-0,03		
323,15	31,135	0,2940	0,7109	+-0,01	+-0,03		
323,15	32,790	0,3338	0,7373	+-0,01	+-0,03		
323,15	35,321	0,4028	0,7772	+-0,01	+-0,03		
323,15	36,276	0,4316	0,7873	+-0,01	+-0,03		
323,15	38,085	0,4872	0,8100	+-0,01	+-0,03		
323,15	39,341	0,5314	0,8254	+-0,01	+-0,03		
323,15	40,160	0,5513	0,8326	+-0,01	+-0,03		
323,15	40,612	0,5688	0,8410	+-0,01	+-0,03		
323,15	42,049	0,6145	0,8569	+-0,01	+-0,03		
323,15	44,916	0,6989	0,8890	+-0,01	+-0,03		
323,15	45,943	0,7290	0,8991	+-0,01	+-0,03		
323,15	47,334	0,7730	0,9160	+-0,01	+-0,03		

KDB calculation model

- 순수성분 물성 계산 프로그램
 - ◆ Source code 및 사용 예제 제공(Fortran 77)
 - ◆ Manual : PDF format
 - ◆ Heat of vaporization, vapor pressure, heat capacity, viscosity, thermal conductivity, surface tension
 - KDB correlation equation : KDB data 이용
 - Poling et al., “Properties of Gases and Liquids”, 5th ed. 의 모델 이용 : 16개 모델

KDB calculation model

The screenshot shows two browser windows. The left window displays the KDB Home Page (Korea thermophysical properties Data Bank) with a navigation menu and a list of thermophysical properties. The right window displays a PDF manual for the KDB_CPG module, detailing the theory for heat capacity of ideal gas and the KDB routines for calculation.

KDB Home Page - Microsoft Internet Explorer
 주소(D) http://www.cheric.org/kdb/index.html

KDB
 Korea thermophysical properties Data Bank
 2002. 7.8 (Mon)

- General DB
- Hydrocarbons
- Polymers
- Electrolytes

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■ Fortran source code for calculation obtained in the following table.
 ■ Fortran files in File Name column proposed by various researchers
 ■ Example Files describe how to use
 ■ Manuals (PDF file) explain the subroutine, and pure properties and supplied by KDB

Thermophysical Properties
Heat of Vaporization
Vapor Pressure
Ideal Gas Heat Capacity
Liquid Heat Capacity
Gas Viscosity
Liquid Viscosity
Gas Thermal Conductivity
Liquid Thermal Conductivity
Surface Tension
Liquid Molar Volume
SRK EoS

http://www.cheric.org/kdb/calmodule/file/manual/KDB_CPG.pdf - Microsoft Internet Explorer
 주소(D) http://www.cheric.org/kdb/calmodule/file/manual/KDB_CPG.pdf

126%

1. Theory for Heat Capacity of Ideal Gas

1) KDB correlation equation (HC_CPGEQN)

Polynomial equation is used for Heat capacity of ideal gas.

$$C_p^0(T) = \sum_{i=0}^4 A_i T^i \quad (1)$$

where, T is Kelvin and $C_p^0(T)$ is kJ/kg-mol.K.

2. KDB Routines for Calculation of Ideal Gas Heat Capacity

KDB Ideal gas heat capacity calculation subroutine contain a KDB correlation equation.

Subroutine Name	Description	Required Common Blocks
HC_CPGEQN	KDB correlation equation	HC_KCPG

1) HC_CPGEQN

- Usage : CALL HC_CPGEQN(ICN,T,HVP,IST)
- Arguments
 - ICN : Component ID number (1-50) to calculate heat of vaporization (integer, input)

KDB management tool

- General Data

- ◆ Dimension
- ◆ Unit
- ◆ Journal
- ◆ Reference
- ◆ Atom

The screenshot shows the KDBMan software interface. On the left, a 'References' table is visible with the following data:

ID	Reference
1	Smith, J. M.
2	Prausnitz,
3	Sandler, S.
4	Pitzer, K. S.
5	Tester, J. W.
6	Prigogine,
7	Hill, T. L.,
8	Hill, T. L.,
9	Guggenhe
10	Allen, M. P.
11	Bondi, A.

The 'Form1' dialog box is open, showing the details for the selected reference (ID 1). The form contains the following fields and values:

- Reference: 1
- Reference Type: Book
- Category: General
- General Reference (TEXT BOOK)
- Keywords: (empty)
- [Authors]:

1	J	M	Smith
2	H	C	Van Ness
3	M	M	Abott
4			
5			
- [Commands]: Save (F2), Save and Exit (F3), Exit (F10), Previous, Next
- Title: Introduction to Chemical Engineering Thermodynamics
- Sub Title: (empty)
- Edition: 5th
- [Journal]:

Journal	cmbJournal
Volume	(empty)
- [Book]:

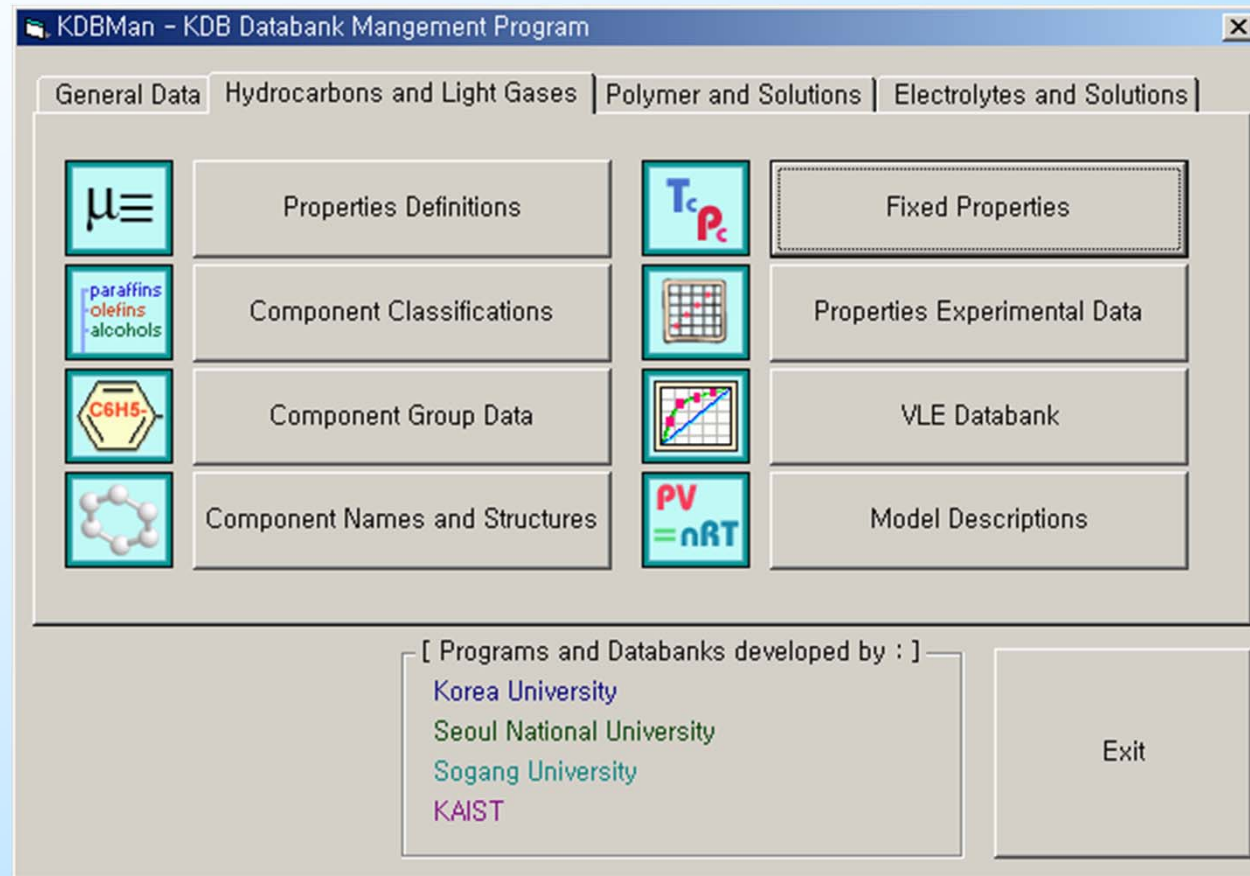
Press	McGraw-Hill
Location	New York
- Page: (empty)
- Year: 1996
- Note: Classical text book on chemical engineering thermodynamics
- Ref. Str.: Smith, J. M., H. C. Van Ness and M. M. Abott, 'Introduction to Chemical Engineering Thermodynamics', 5th ed., McGraw-Hill, New York

At the bottom of the form, there are instructions:

- [1] Author Names must be typed without period (.) (for example: J F Kennedy)
- [2] Titles and Sub-Titles must be typed without (") (quotation)
- [3] Editions of the books must be typed as 1st, 2nd, 3rd, 4th,

KDB management tool

- Hydrocarbons and Light Gases



- Hydrocarbons and Light Gases

- ◆ Properties Definition

The image shows two overlapping windows from a software application. The background window is titled 'Hydrocarbons - Properties' and contains a table of property definitions. The foreground window is titled 'HC - Editing Properties Definitions' and is used for editing a specific property.

Hydrocarbons - Properties

ID	Code	Name
1	WTM	Molecular Weight
2	TB	Normal Boiling Point
3	TF	Freezing Point
4	TC	Critical Temperature
5	PC	Critical Pressure
6	VC	Critical Volume
7	ZC	Critical Compressibility Factor

HC - Editing Properties Definitions

Property Code: 1 WTM

Property Name: Molecular Weight

Component Type: For Hydrocarbons and Light Gases

Property Type: Pure Component Fixed Property

Coherent Property

Property Dimension: Dimensionless

[Default Units of Measure]

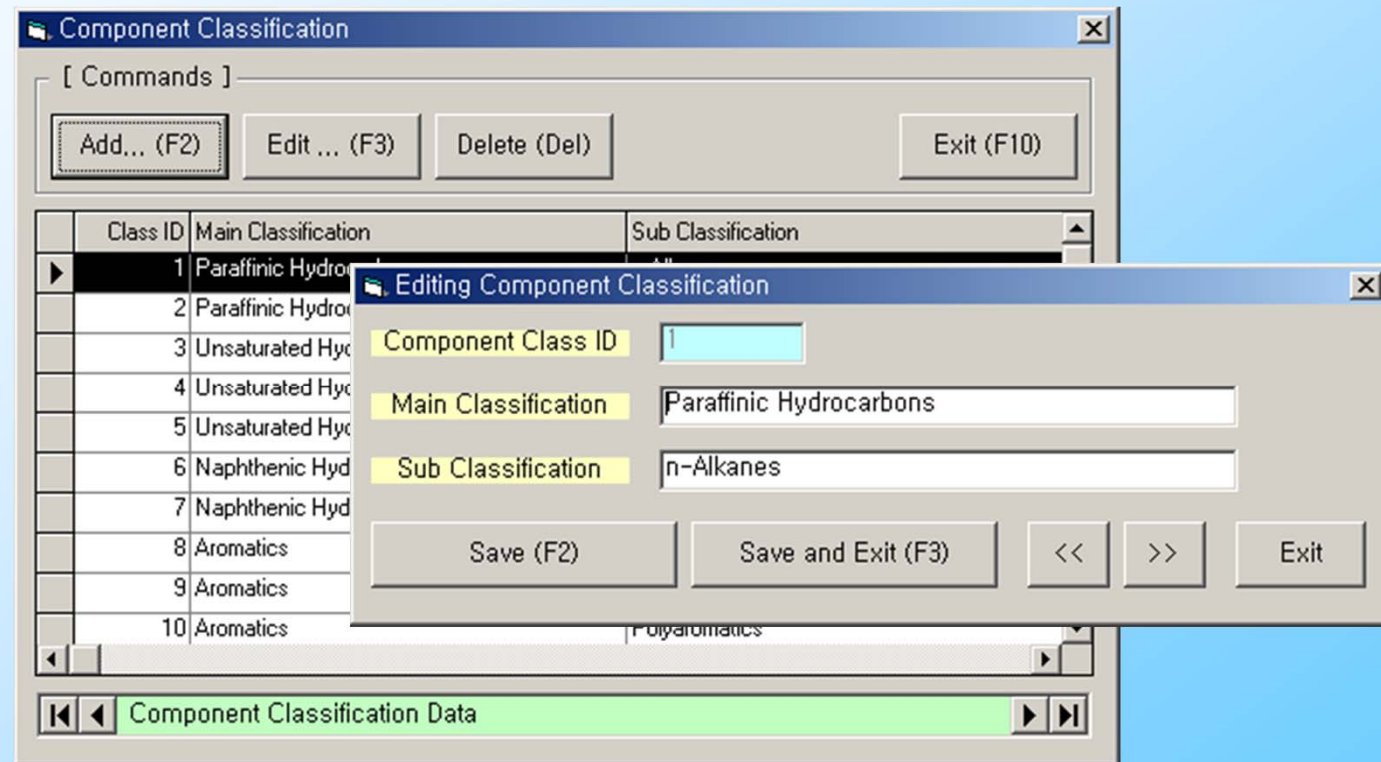
	SI	Metric	English
Molar			
Weight			

Definition

The weight of one mole of specified molecule in grams, (g/g-mole or kg/kg-mol)
The value is calculated from the atomic content of the molecule and the atomic weight of the elements given in the IUPAC periodic table of the elements.

Buttons: Save (F2), Save and Exit (F3), <<, >>, Exit

- Hydrocarbons and Light Gases
 - ◆ Component classifications



- Hydrocarbons and Light Gases
 - ◆ Component Group Data

The screenshot displays a software interface with a 'Form1' dialog box overlaid on a main window. The main window contains a table with the following data:

Group ID	Classification
1	PARAFFINIC
2	PARAFFINIC
3	PARAFFINIC
4	PARAFFINIC
5	PARAFFINIC
6	NAPHTHEN
7	NAPHTHEN
8	NAPHTHEN
9	UNSATURA
10	UNSATURA
11	UNSATURATED

The 'Form1' dialog box is titled 'Form1' and contains the following fields and buttons:

- Group ID: 1
- Group Classification: PARAFFINIC
- Group Name: CH4 (METHANE)
- Group Mol. Wt.: 16.0426
- Formula: CH4
- Buttons: Save (F2), Save and Exit (F3), <<, >>, Exit

The dialog box also has a status bar at the bottom with the text 'Component Group Data' and navigation arrows.

- Hydrocarbons and Light Gases

- ◆ Component Name

The screenshot displays a software interface for editing component names and formulas. On the left, a table lists components with their IDs and names. The main window, titled 'Editing Component Names and Formulas', provides a detailed view for component 1, Methane.

Comp.ID	Component Name
1	METHANE
2	ETHANE
3	PROPANE
4	N-BUTANE
5	N-PENTANE
6	N-HEXANE
7	N-HEPTANE
8	N-OCTANE
9	N-NONANE
10	N-DECANE
11	N-UNDECANE

Editing Component Names and Formulas

[General Information]

- Component ID: 1
- Component Name: METHANE
- Synonym 1: METHYL HYDRIDE
- Synonym 2: MARSH GAS
- Synonym 3:
- Abbreviated Name: NC01
- CA Name:
- CA Registry No.: 74-82-8
- Formula: CH₄ (Long Form) CH₄
- Classification: Paraffinic Hydrocarbons - n-Alkanes
- Molecular Weight: 16.0426
- No. of Carbons: 1

CH₄

Buttons: Edit Structural Groups ..., Save (F2), Save and Exit (F3), <<, >>, Exit

- Hydrocarbons and Light Gases

- ◆ Fixed Properties

The image displays two screenshots of the 'Component Fixed Properties' software interface, showing the configuration for Methane (CH₄).

Left Screenshot: Basic Properties Page 1

- Component: 1 | METHANE
- METHYL HYDRIDE
- MARSH GAS
- Formula: CH₄
- CAS No.: 74-82-8
- Classification: Paraffinic Hydrocarbons

Property	Value
Molecular Weight	16.0
Boiling Point	11
Freezing Point	9
Triple Point Temp.	90
Triple Point Pres.	11
Critical Temp.	190
Critical Pressure	
Critical Volume	0.0
Critical Comp. (ZC)	0.288

Right Screenshot: Basic Properties Page 2

- Component: 1 | METHANE
- Formula: CH₄ | CH₄
- CAS No.: 74-82-8
- Classification: Paraffinic Hydrocarbons (n-Alkanes)

Property	Equation	A	B	C	D	E	F	G	Coef. Ref.	Exp. Ref.	Ref...
Vapor Pressure	Vapor Pressure			2.664952E+01	2.048824E-05						Ref...
Ideal Gas Heat Capacity	Ideal Gas Heat Capacity										Ref...
Liquid Heat Capacity	Liquid Heat Capacity										Ref...
Gas Viscosity	Gas Viscosity										Ref...
Liquid Viscosity	Liquid Viscosity										Ref...
Gas Thermal Conductivity	Gas Thermal Conductivity										Ref...
Liquid Thermal Conductivity	Liquid Thermal Conductivity										Ref...

Buttons: Update Current Page, Save To Databank, Save As Text File ..., Exit

- Hydrocarbons and Light Gases
 - ◆ Properties Experimental Data

The screenshot displays two overlapping windows from a software application. The background window, titled 'Properties Experimental', contains a table of components and an 'Edit ... (F3)' button. The foreground window, titled 'Form1', shows a form for editing experimental data for Methane.

Properties Experimental Window:

Comp.ID	Component
1	METHANE
2	ETHANE
3	PROPANE
4	N-BUTANE
5	N-PENTANE
6	N-HEXANE
7	N-HEPTANE
8	N-OCTANE
9	N-NONANE
10	N-DECANE
11	N-UNDECANE

Form1 Window:

Component: METHANE
 Property: All Data

Buttons: Add ... (F2), Edit ... (F3), Delete ... (Del), Exit (F10)

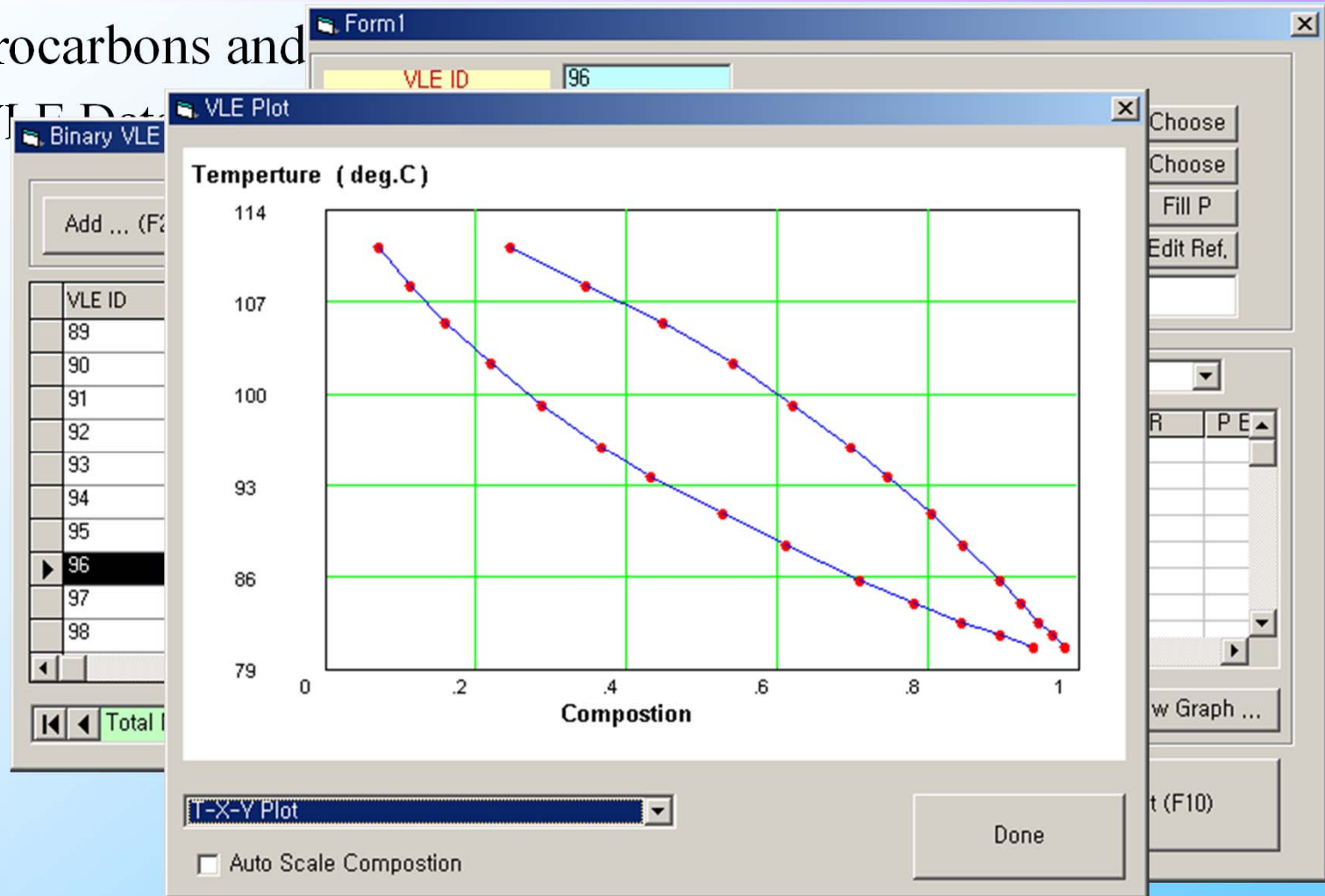
Property	DB Default Value	Default Unit	Reference	Value in Original	Unit	Accuracy
TB	1.11600E+02	K	14	111.6	K	
TB	1.11670E+02	K	17	111.67	K	
TB	1.11410E+02	K	16	-161.74	C	
TF	9.07000E+01	K	14	90.7	K	
TF	9.06900E+01	K	17	90.69	K	
TF	9.06300E+01	K	16	-182.52	C	
TF	9.06600E+01	K	16	-182.49	C	
TF	9.06600E+01	K	16	-182.49	C	
TC	1.90564E+02	K	46	190.564	K	+0.015
TC	1.90400E+02	K	14	190.4	K	

Form1 Window Footer: Pure Component Fixed Properties Experimental Data Sets

KDB management tool

- Hydrocarbons and

- ◆ VLE Data



활용과 전망

- 대학, 연구소, 산업계에 대한 무료 검색 서비스
 - ◆ KDB web : internet 검색 서비스
 - ◆ Management tool 의 공급
- 지속적인 자료의 축적
 - ◆ 자료의 절대적인 양을 늘임
 - ◆ 정부, 산업체의 연계를 통한 지원 필요
- 독자적 특성 부여를 통한 상업적 활용 가능성