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-DETHERM(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-DETHERM(독일)

- Contents of DETHERM

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

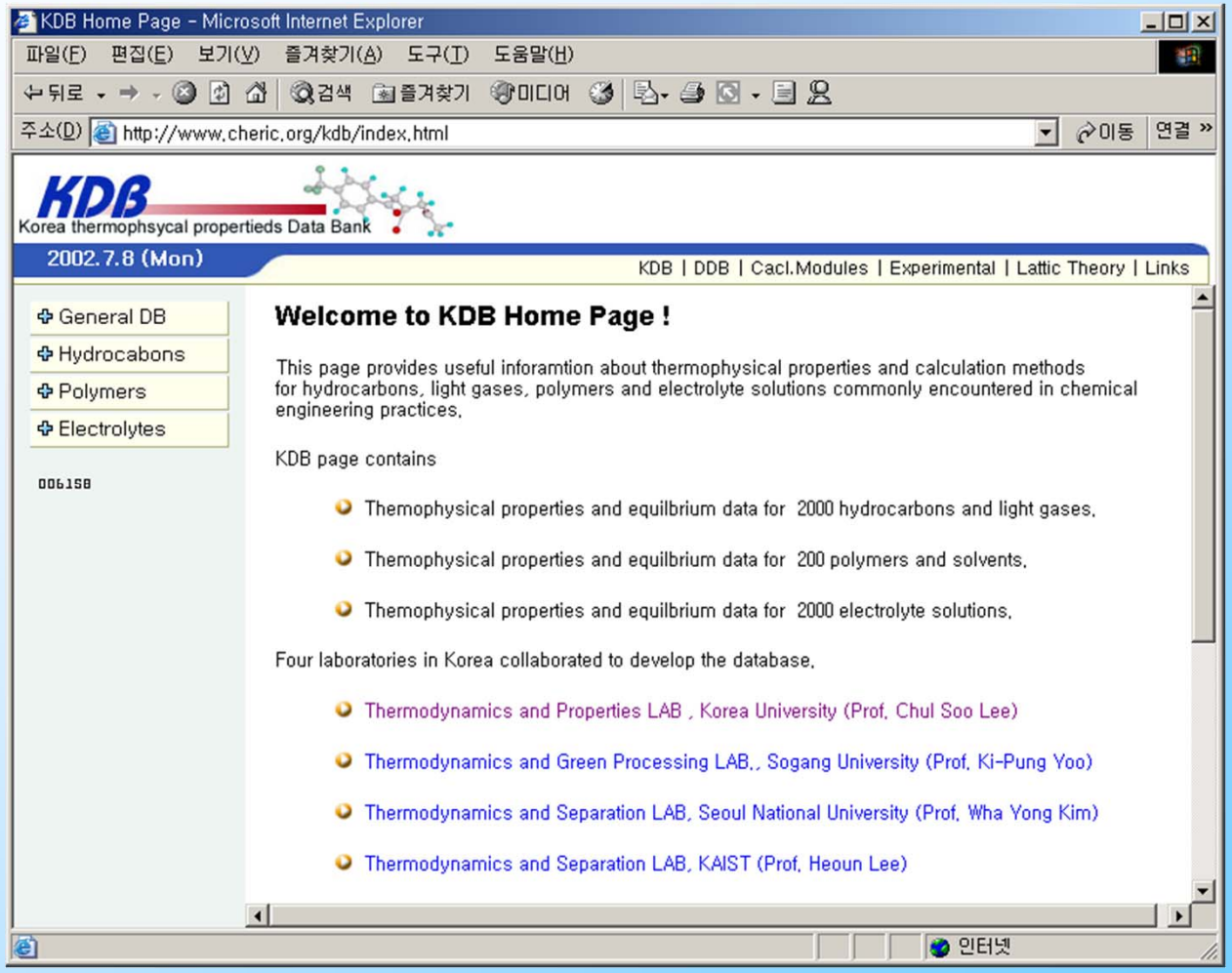
KDB 개발방향

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

KDB 개발 체계

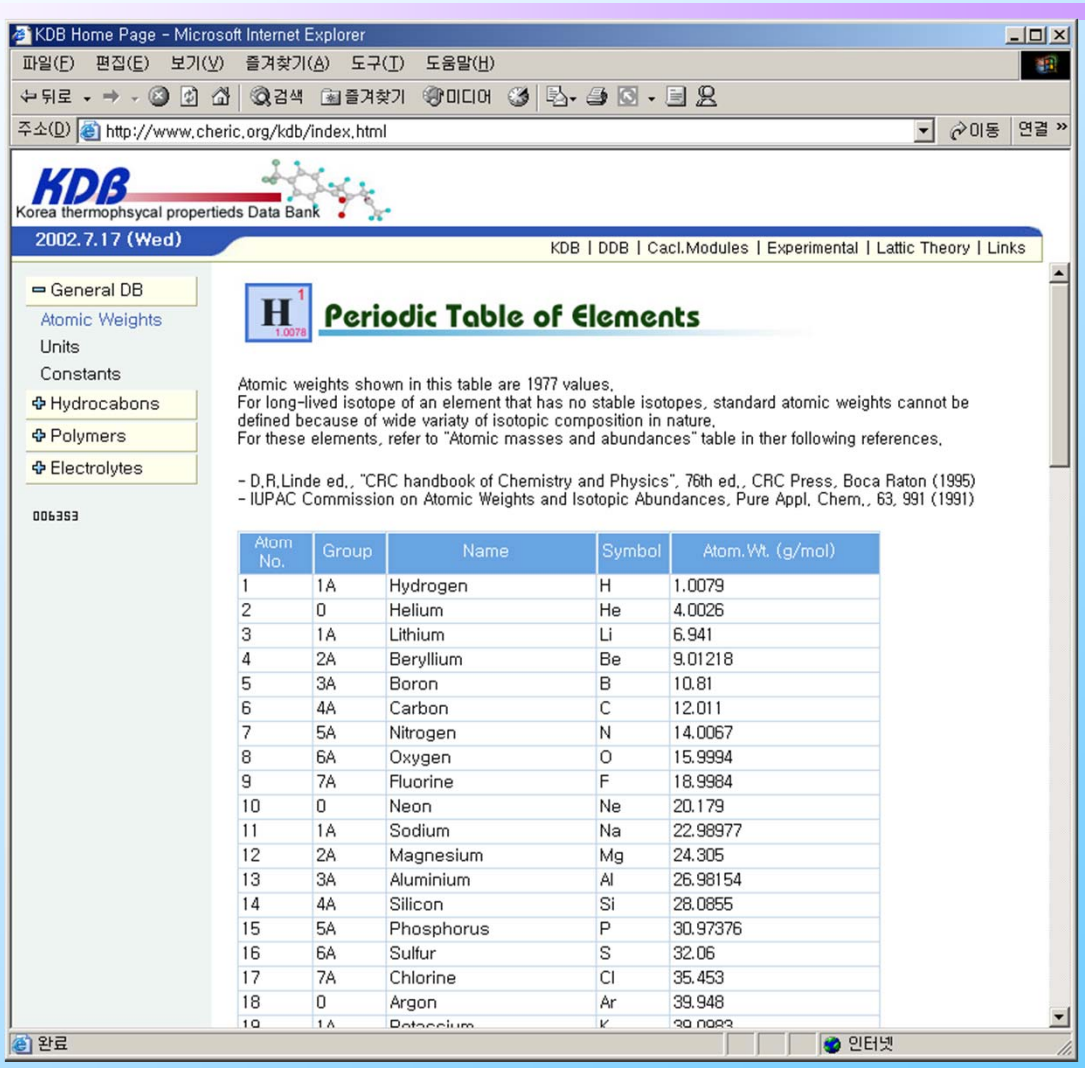
- 고려대학교 화공생명공학과 열역학 및 물성연구실
  - 탄화수소류, 전해질, 고분자계의 열역학 물성 축적
  - 열역학 모델 개발
  - 열역학 물성 계산 프로그램 공급
- 고려대학교 화학공학정보센터
  - Database 관리
  - 인터넷 서비스

KDB WEB Home Page



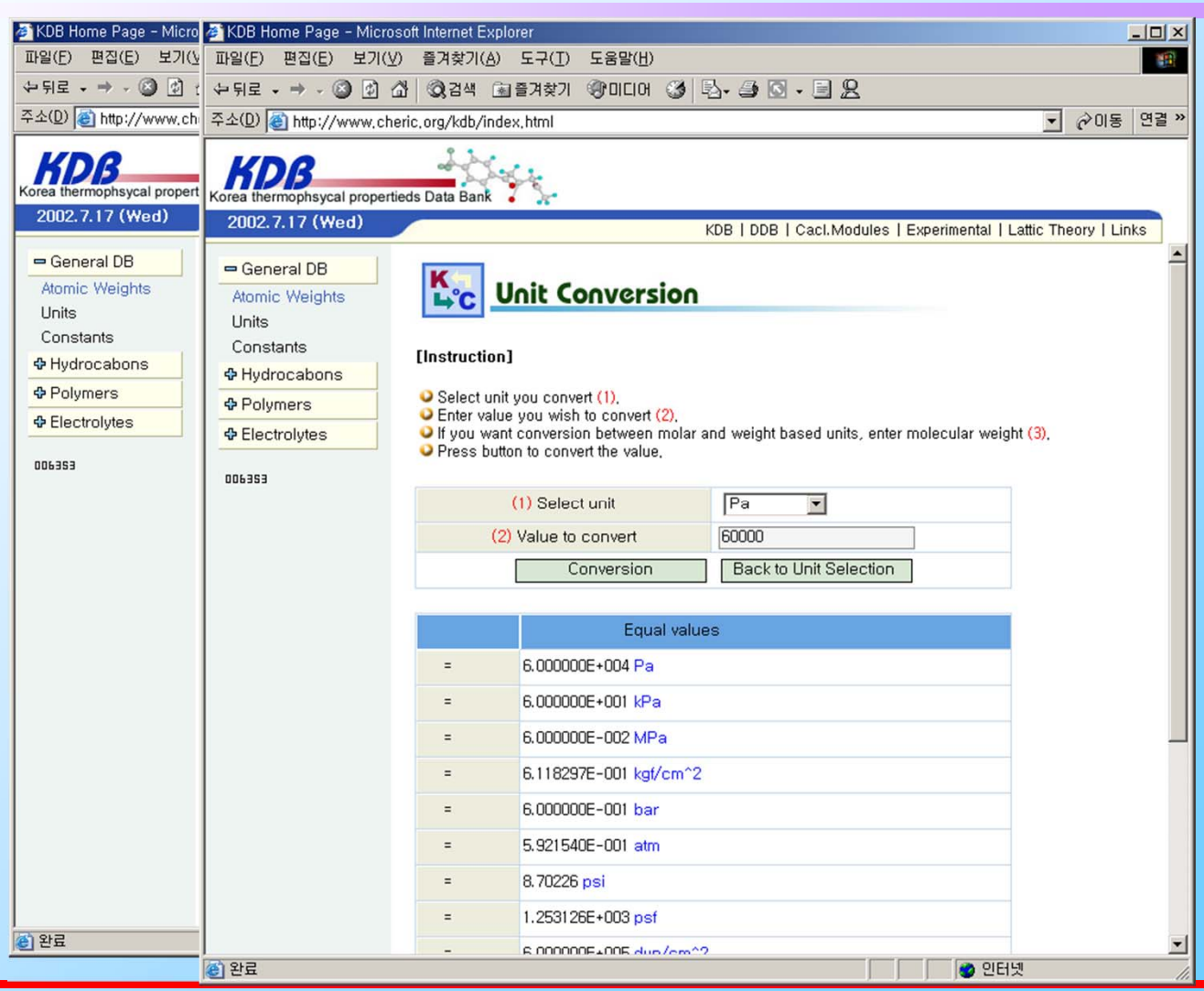
KDB general databank

- 원자량



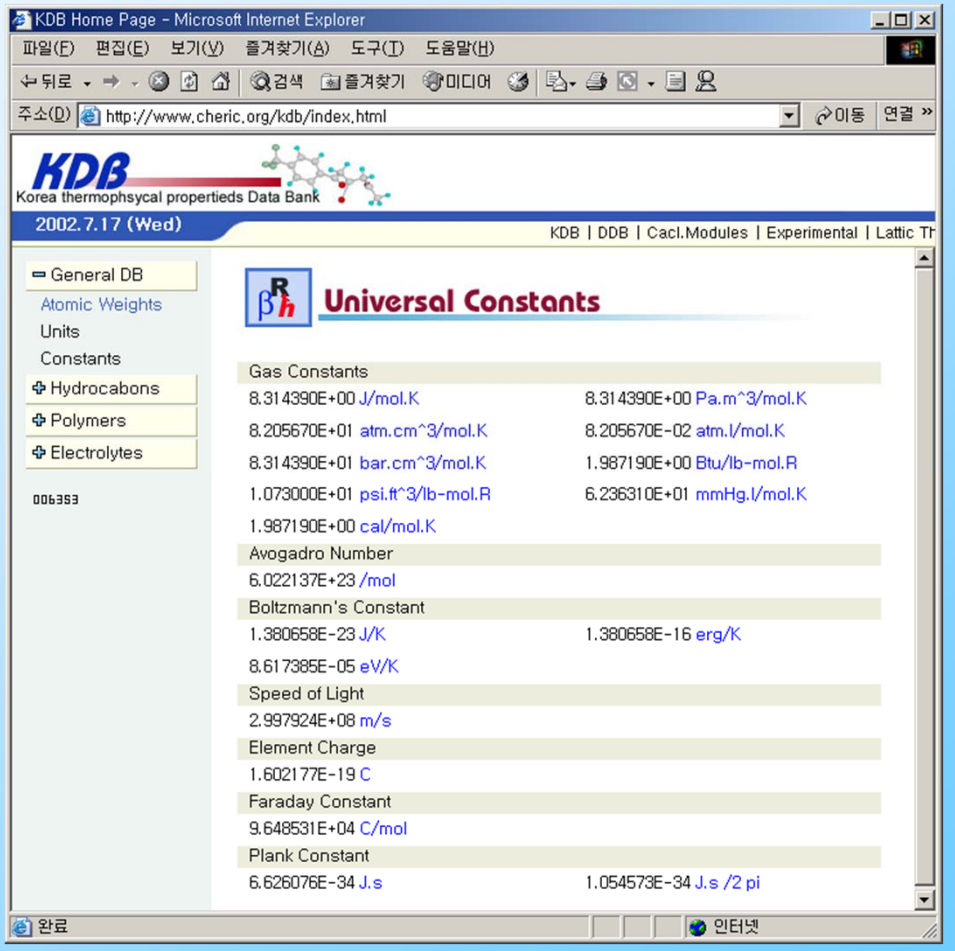
KDB general databank

- Units



KDB general databank

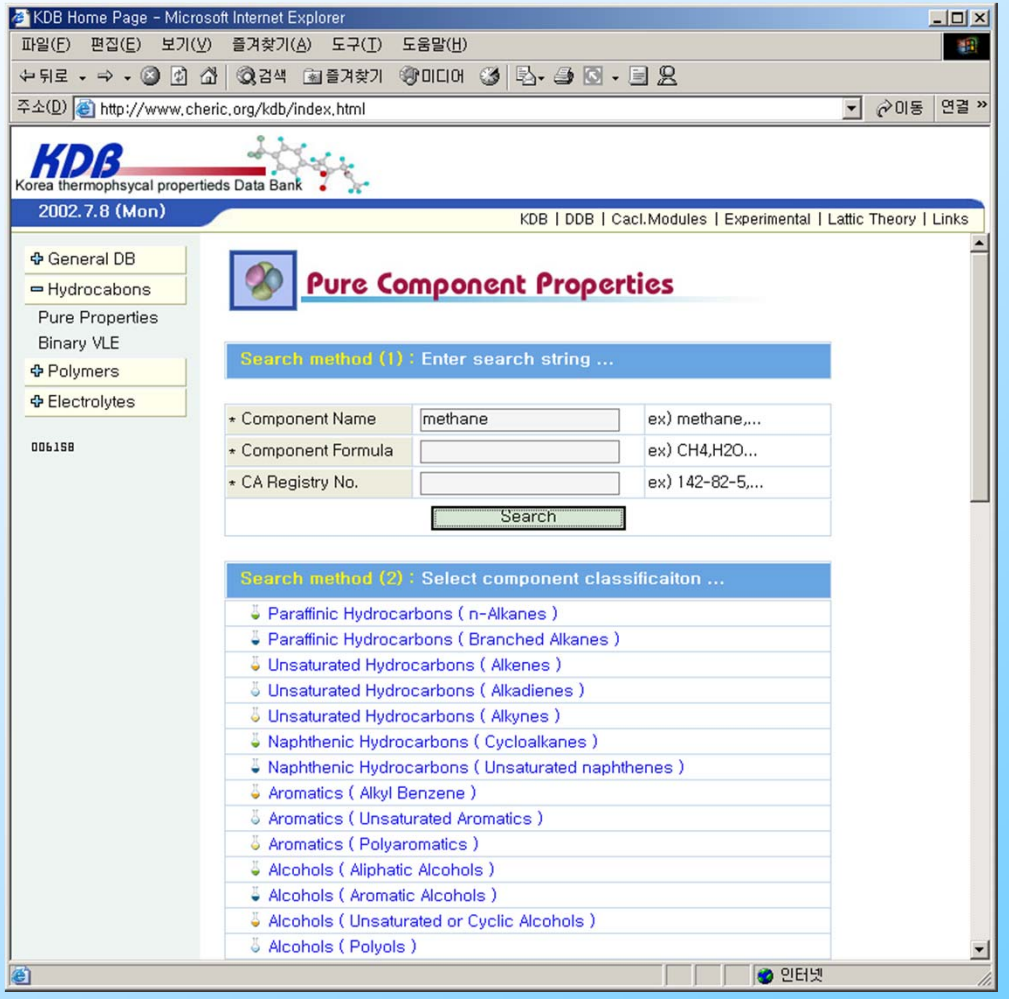
- 상수(Constants)



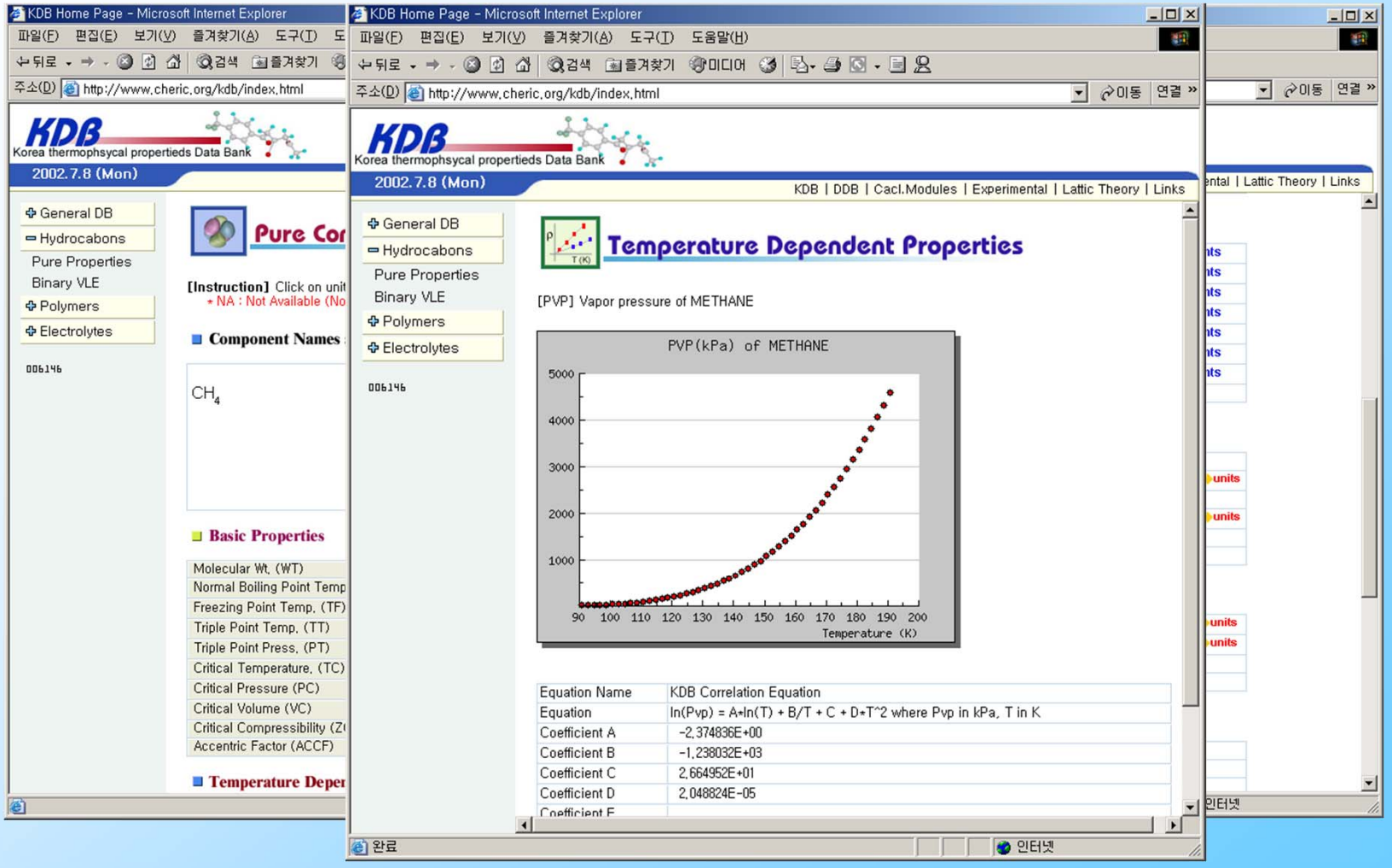
KDB 순수성분 데이터

- 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
파일(F) 편집(E) 보기(V) 즐겨찾기(A) 도구(T) 도움말(H)
뒤로 검색 즐겨찾기 미디어
주소(D) http://www.cheric.org/kdb/index.html
이동 연결
KDB
Korea thermophysical properties Data Bank
2002.7.8 (Mon)
KDB | DDB | Cacl.Modules | Experimental | Lattic Theory | Links
General DB
Hydrocabons
Pure Properties
Binary VLE
Polymers
Electrolytes
006158
Pure Component Properties
Search method (1) : Enter search string ...
* Component Name
methane
ex) methane,...
* Component Formula
ex) CH4,H2O...
* CA Registry No.
ex) 142-82-5,...
Search
Search method (2) : Select component classificaiton ...
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)
인터넷

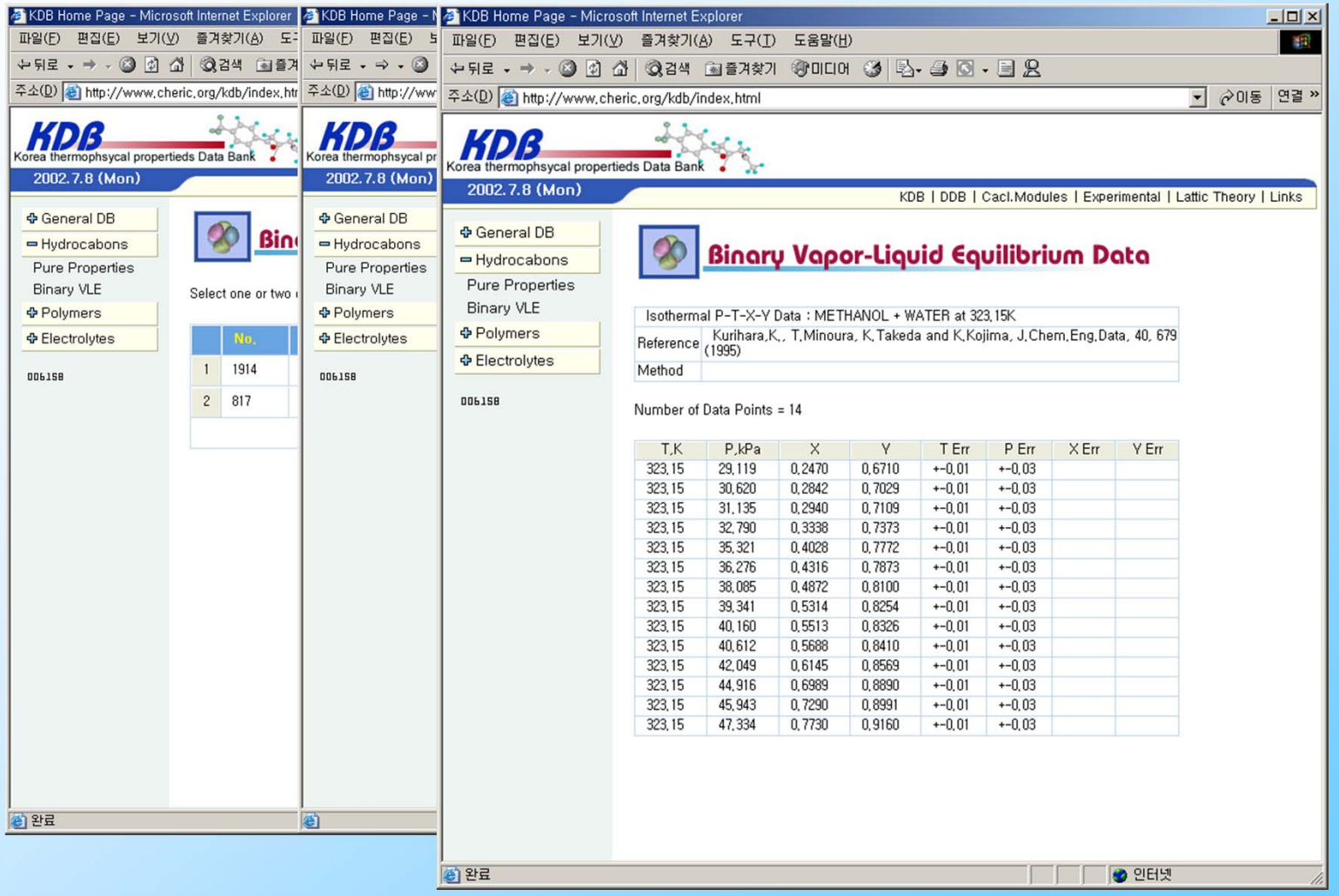
KDB 순수성분 물성


KDB Home Page - Microsoft Internet Explorer
http://www.cheric.org/kdb/index.html
KDB
Korea thermophsycal propertieds Data Bank
2002.7.8 (Mon)
KDB | DDB | Cacl.Modules | Experimental | Lattic Theory | Links
General DB
Hydrocabons
Pure Properties
Binary VLE
Polymers
Electrolytes
006146
Temperature Dependent Properties
[PVP] Vapor pressure of METHANE
PVP(kPa) of METHANE
Temperature (K)
Equation Name KDB Correlation Equation
Equation ln(Pvp) = A+ln(T) + B/T + C + D*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
[Instruction] Click on unit
* NA : Not Available (No
Component Names
CH4
Basic Properties
Molecular Wt. (WT)
Normal Boiling Point Temp
Freezing Point Temp. (TF)
Triple Point Temp. (TT)
Triple Point Press. (PT)
Critical Temperature. (TC)
Critical Pressure (PC)
Critical Volume (VC)
Accentric Factor (ACCF)
완료
인터넷

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)

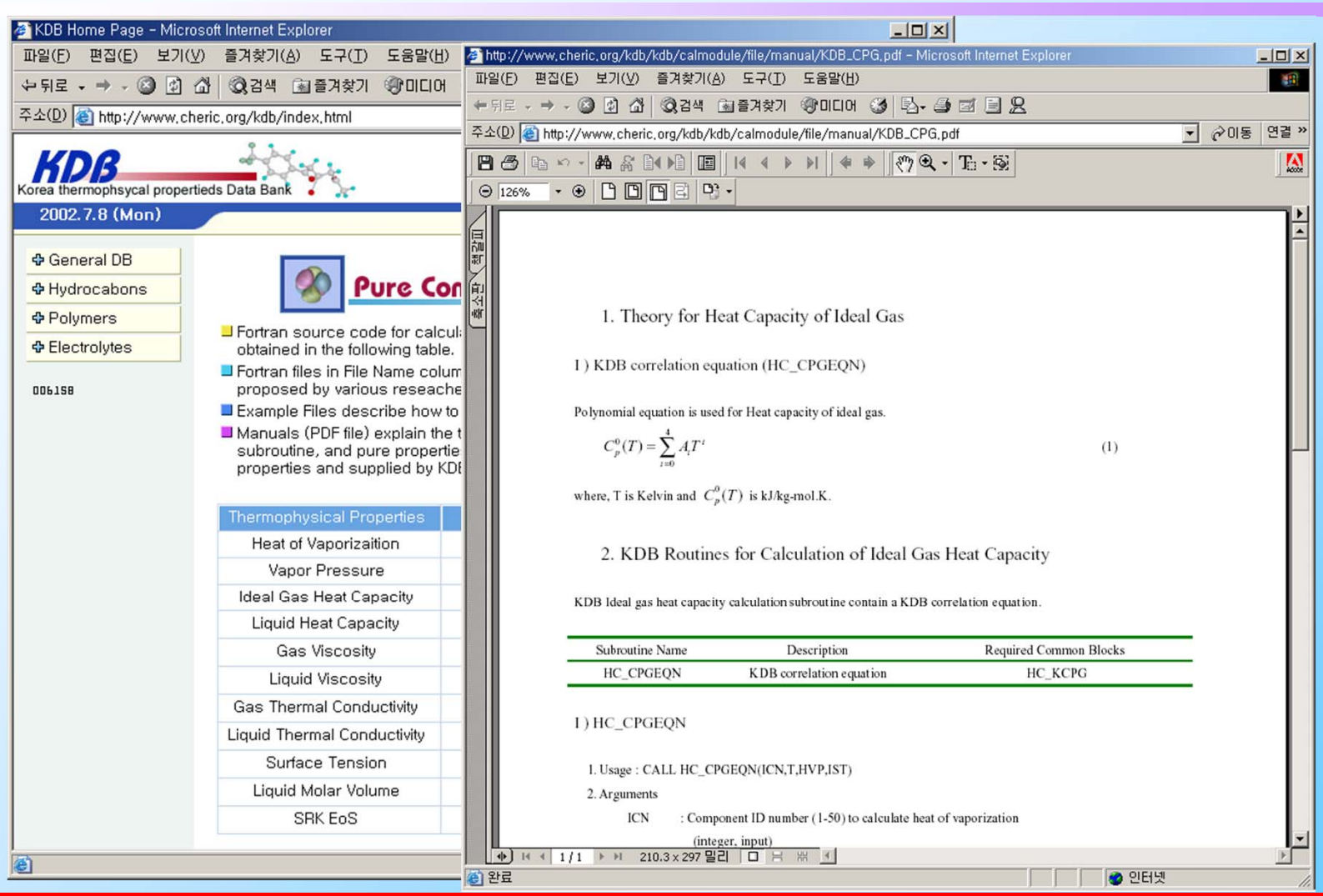
KDB 혼합물 평형 데이터



KDB calculation model

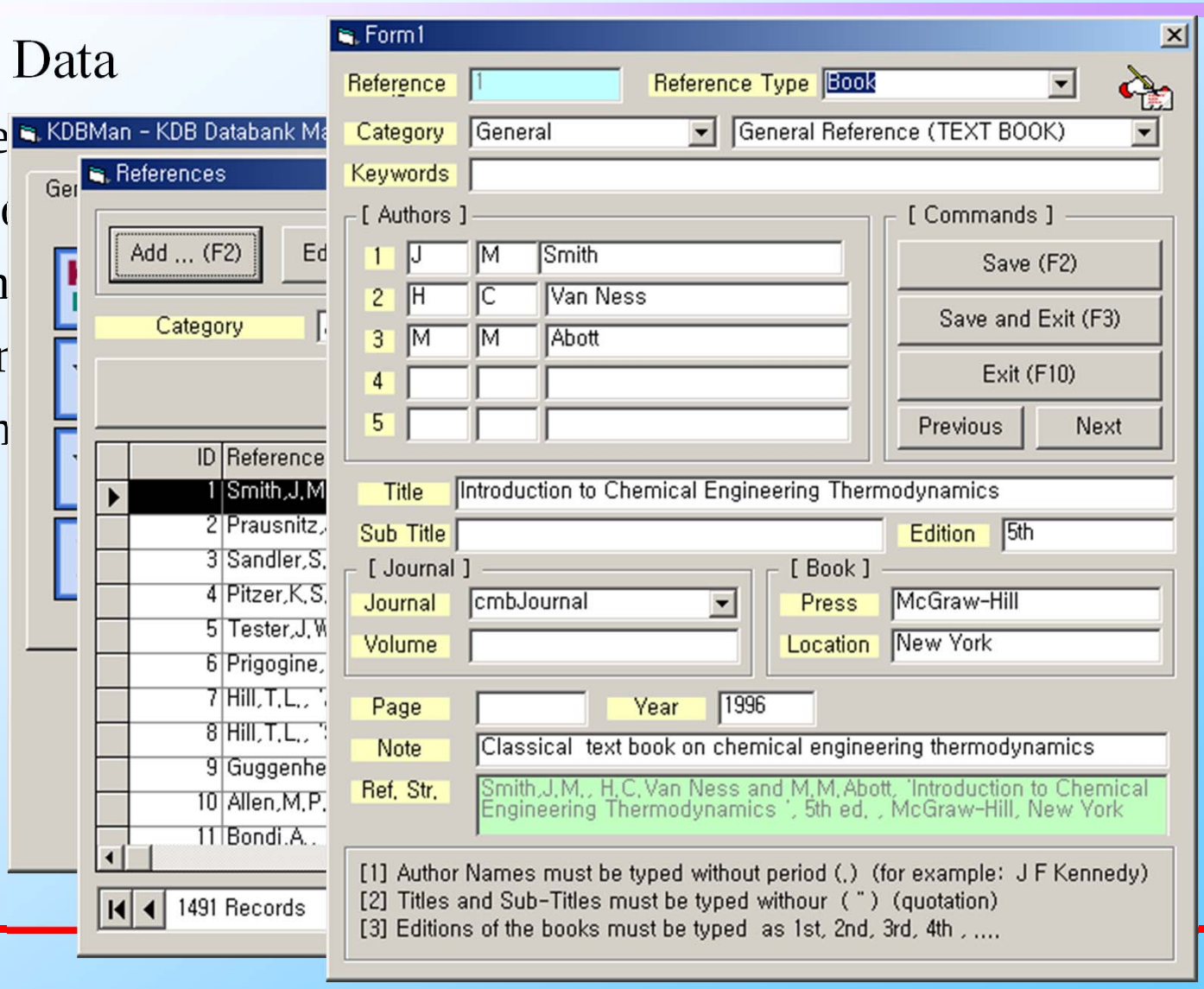
- 순수성분 물성 계산 프로그램
  - Source code 및 사용 예제 제공(Fortran 77)
  - Manual : PDF format
  - Heat of vaporization, vapor pressure, heat capacity, viscosity, thermal conductivity, surface tension
    - KDB correlation equation : KDB data 이용
    - Poling et al., “Properties of Gases and Liquids”, 5th ed. 의 모델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

KDB calculation model



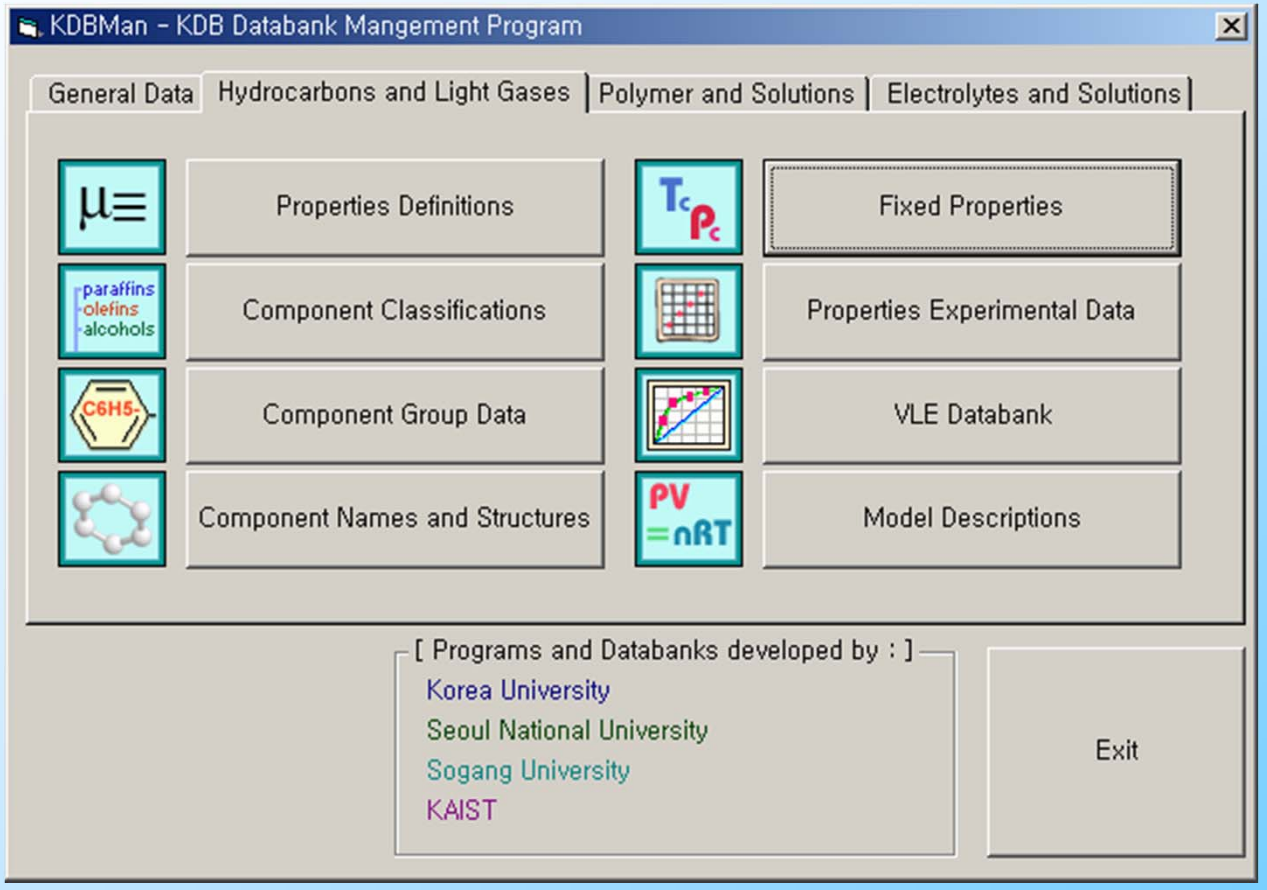
KDB management tool

- General Data
  - Dime
  - Unit
  - Journ
  - Refer
  - Atom

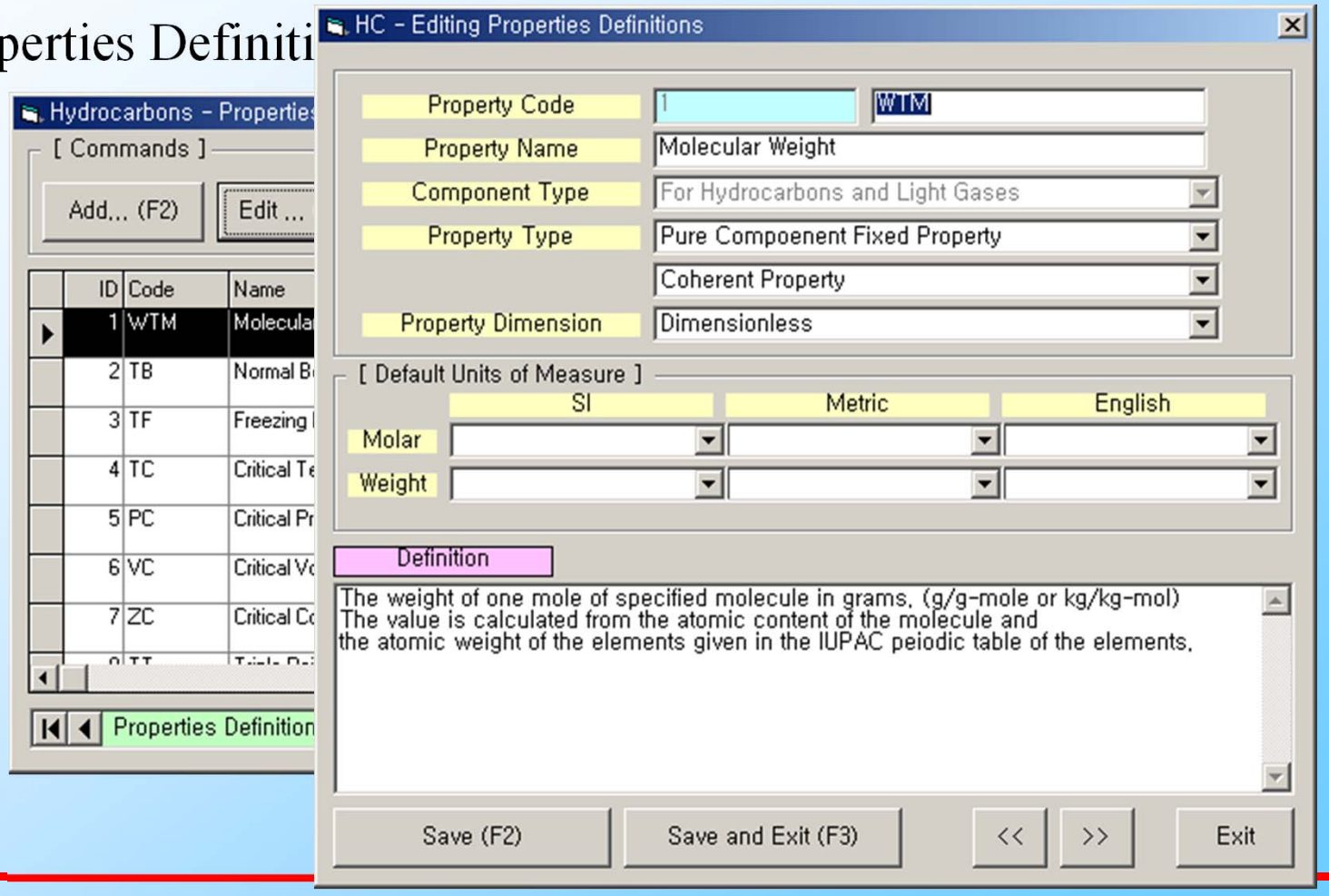


KDB management tool

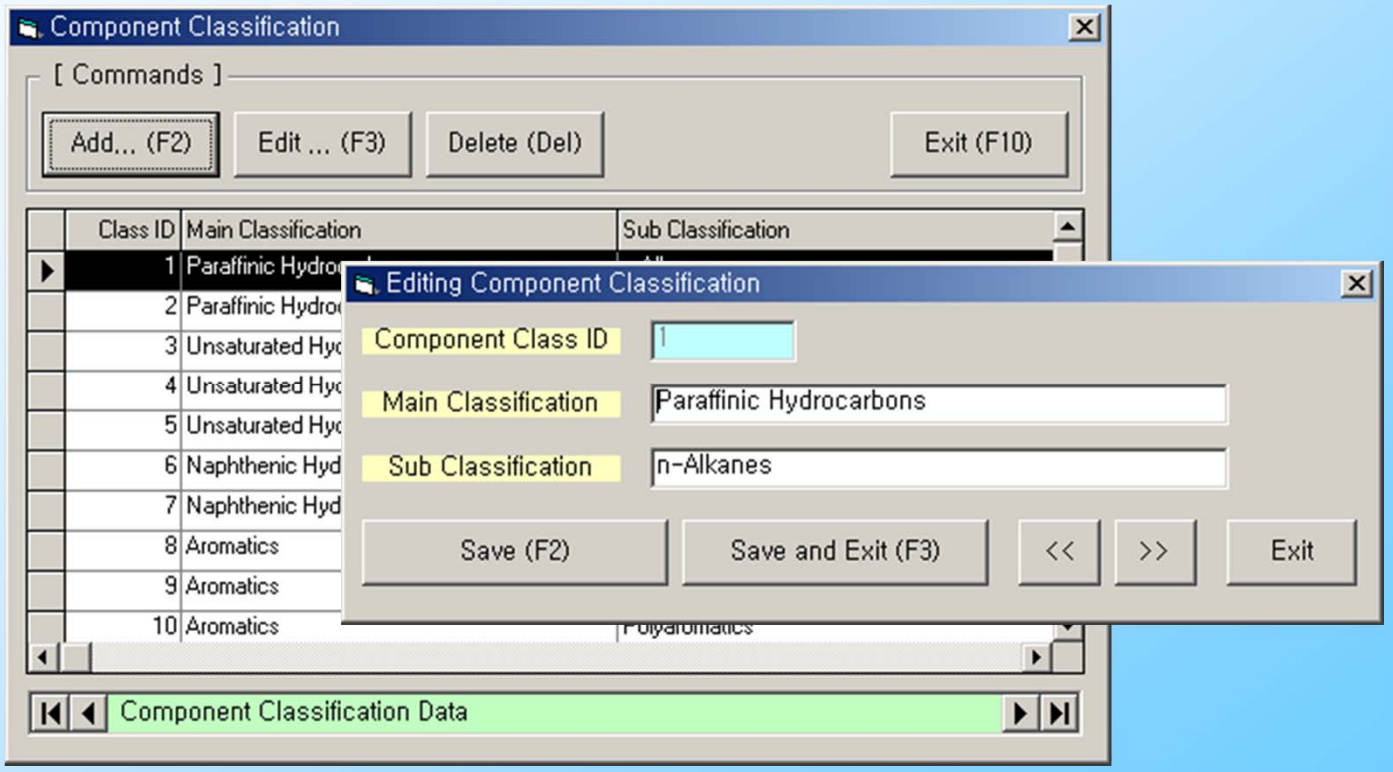
- Hydrocarbons and Light Gases



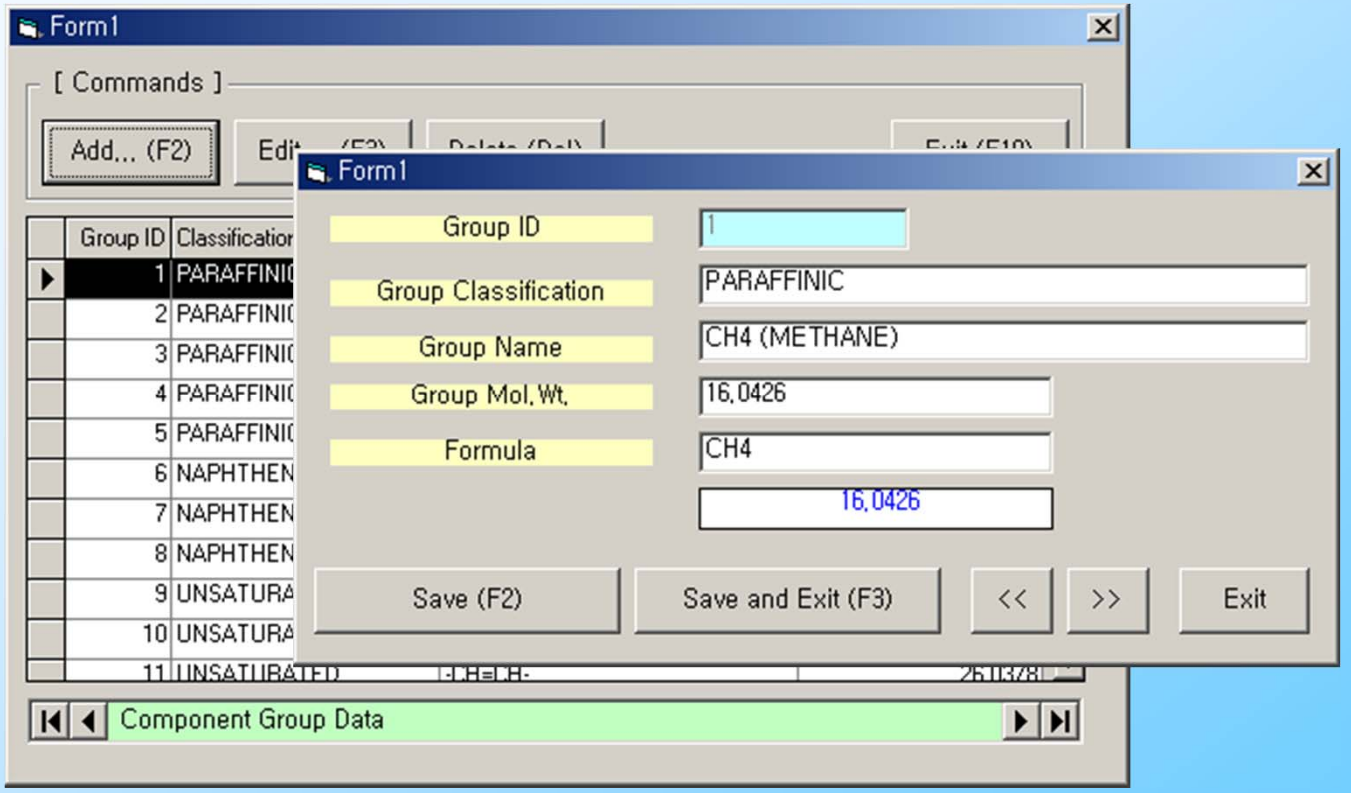
- Hydrocarbons and Light Gases
  - Properties Definiti



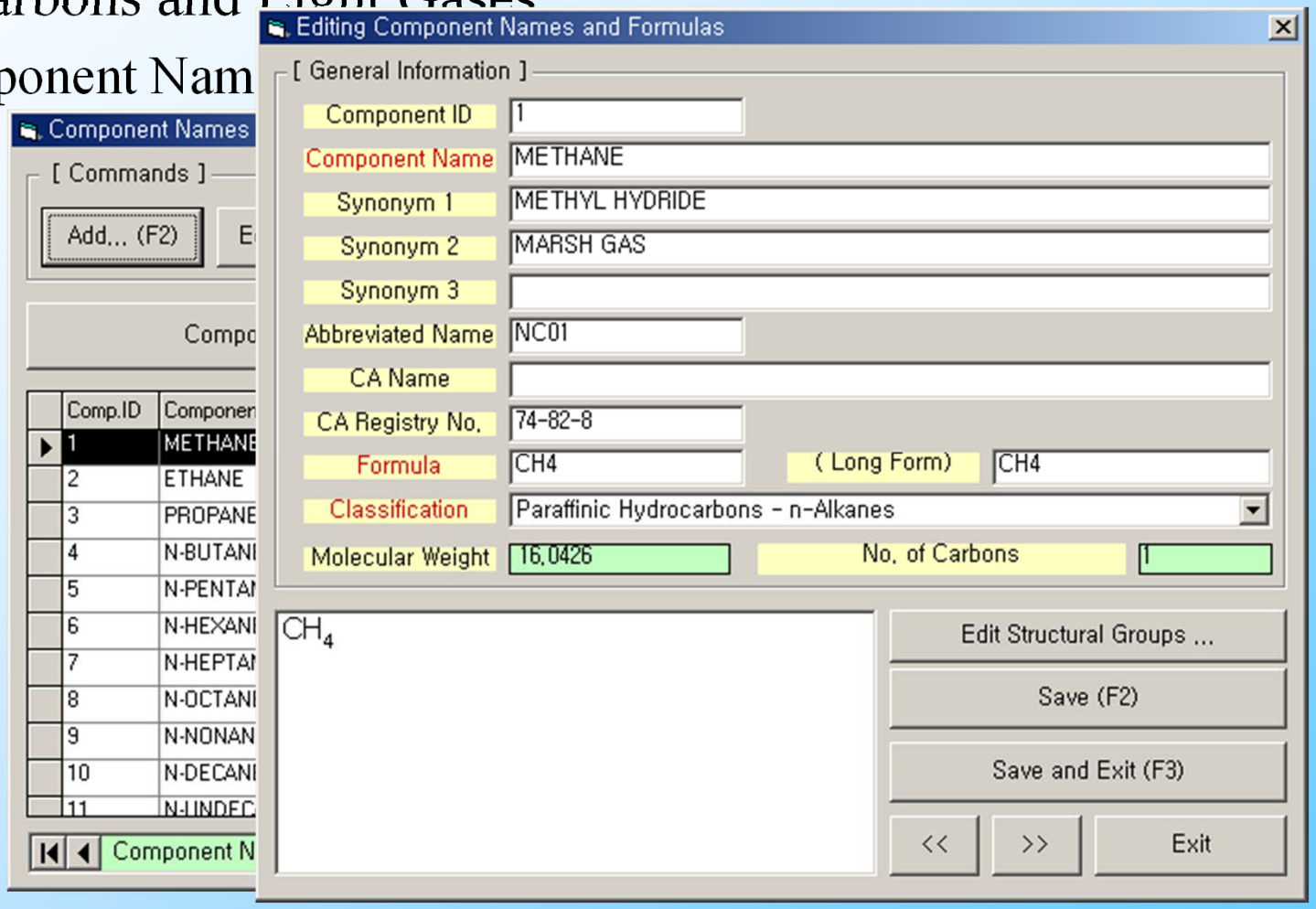
- Hydrocarbons and Light Gases
  - Component classifications



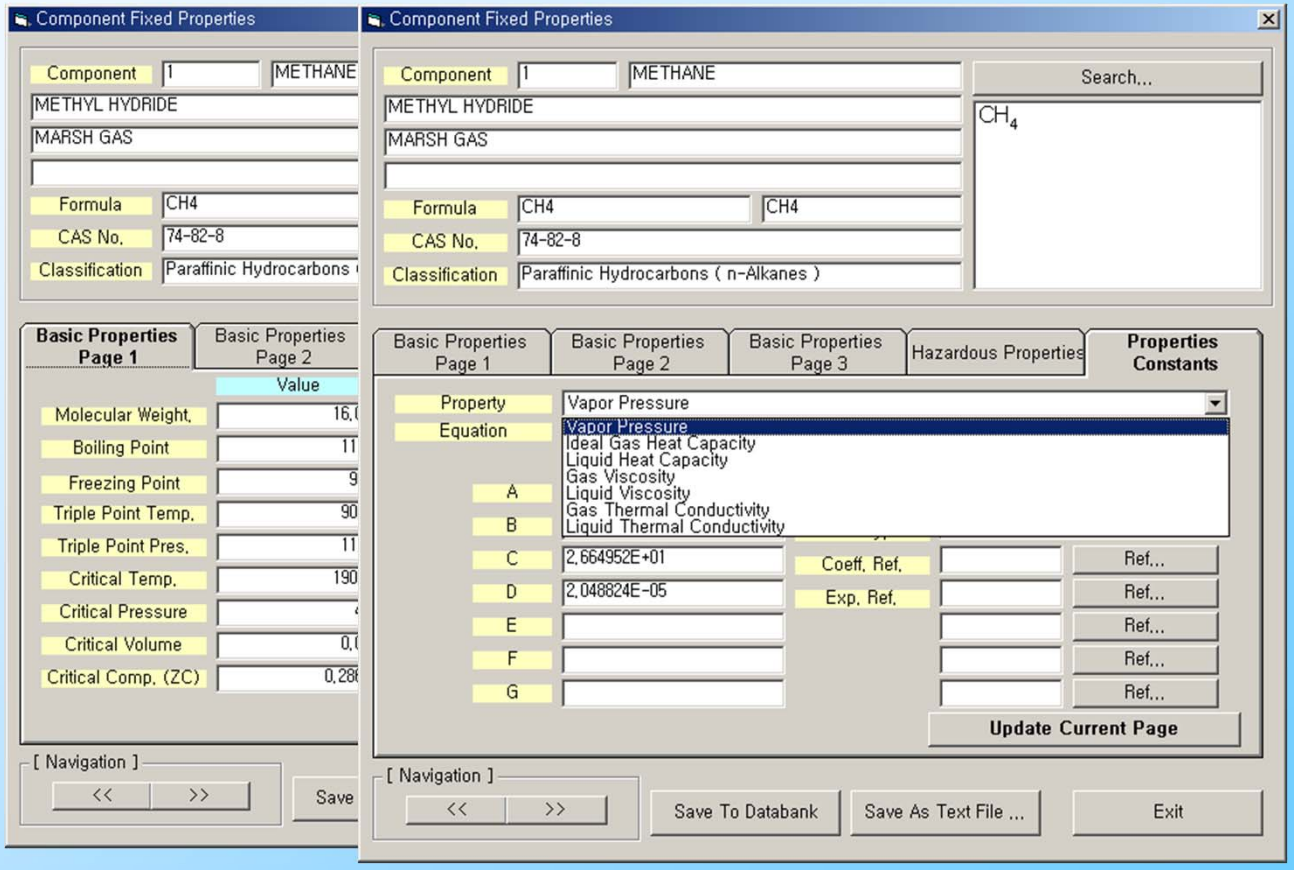
- Hydrocarbons and Light Gases
  - Component Group Data



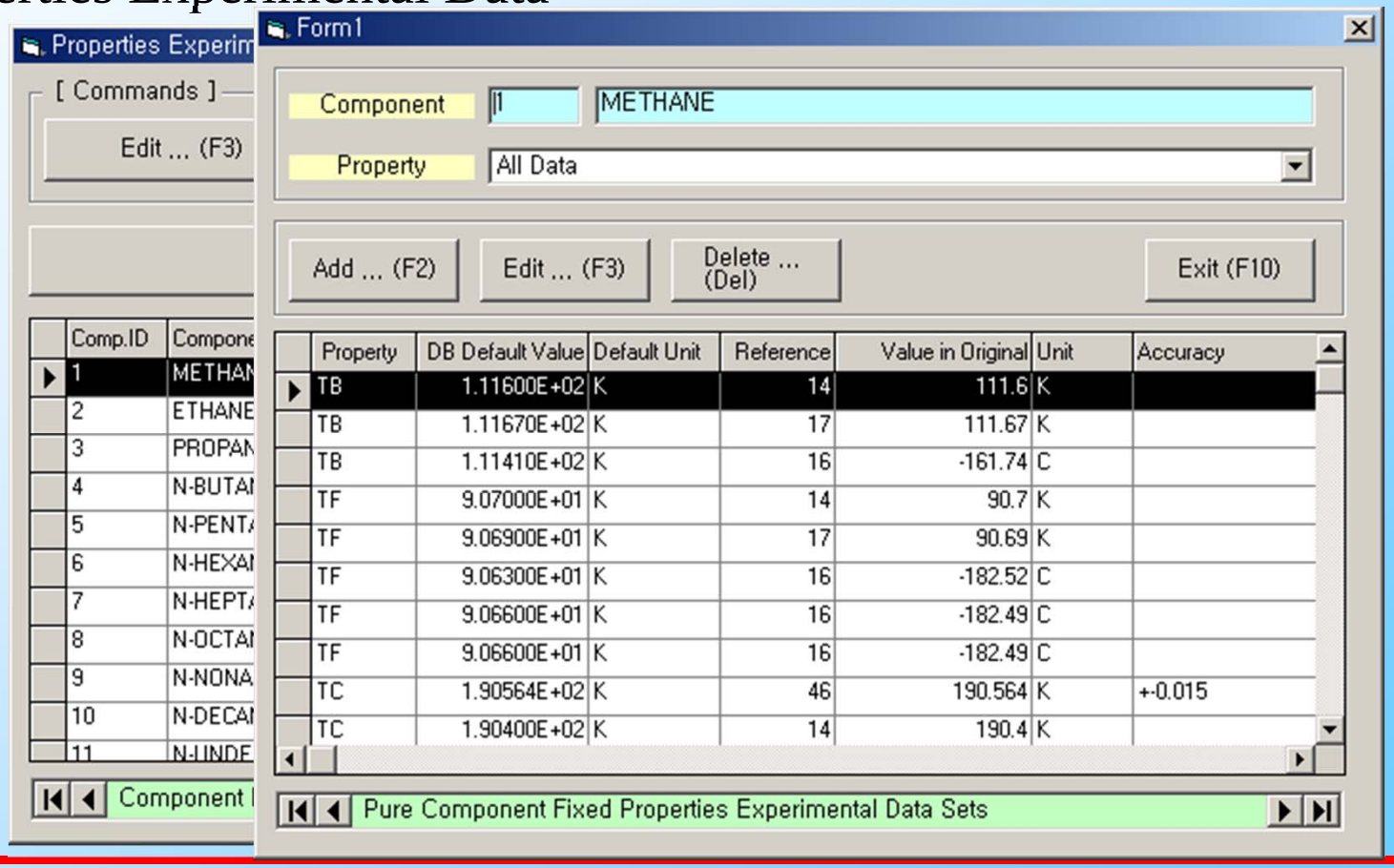
- Hydrocarbons and Light Gases
  - Component Nam



- Hydrocarbons and Light Gases
  - Fixed Properties

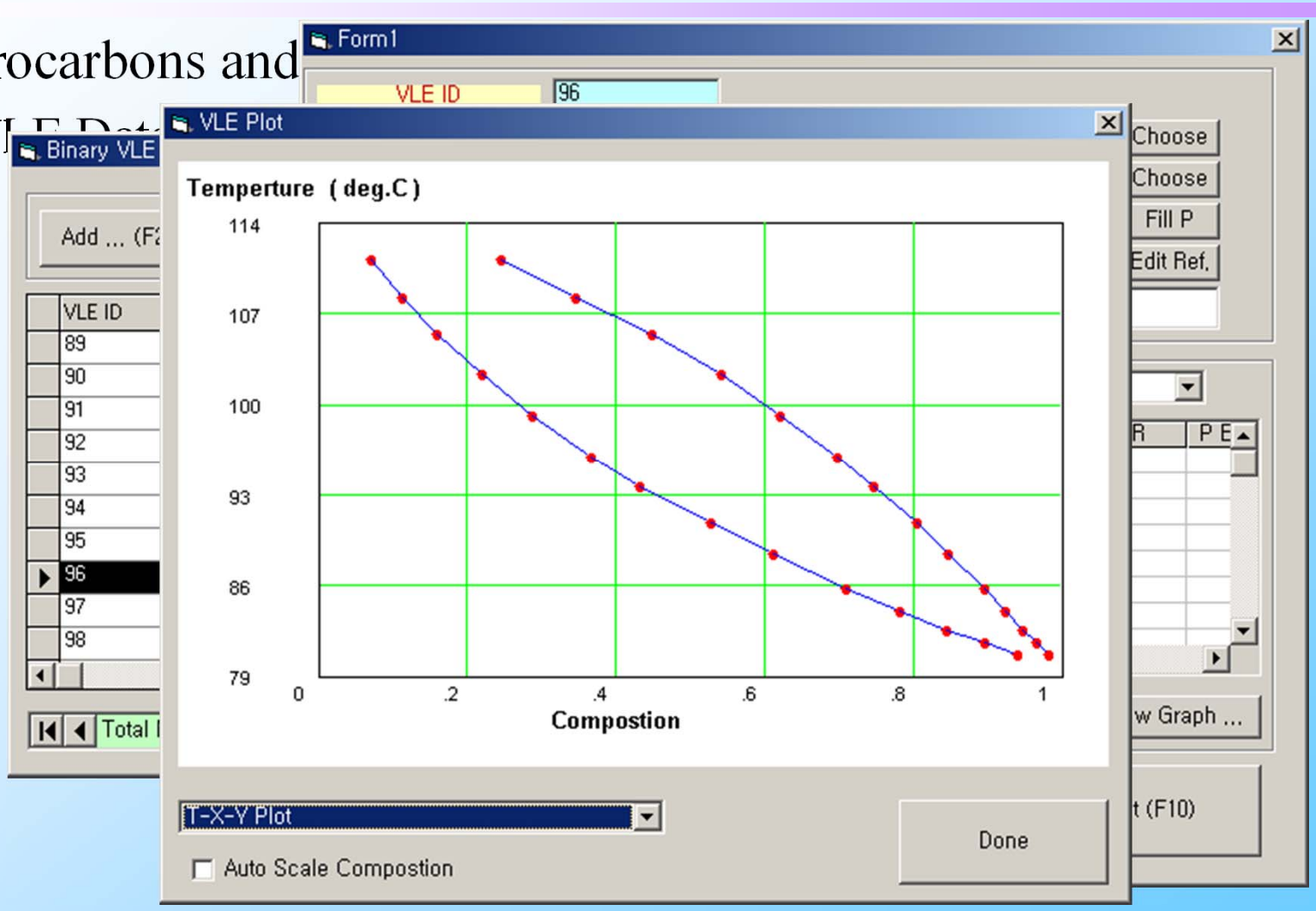


- Hydrocarbons and Light Gases
  - Properties Experimental Data



KDB management tool

- Hydrocarbons and
  - VL



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