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Development and Current Status of the Korea Thermophysical Properties Databank (KDB)[1]

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Physical property data, phase equilibrium data, and predictive models are essential parts of process design and operation. With the support of the Ministry of Commerce, Industry and Energy (MOCIE) of Korea, four universities collaborated to develop a thermophysical property databank and to obtain experimental data. In this paper topics related to the development and use of the thermophysical properties and phase equilibrium database are discussed. The databank contains about 4000 pure components and 5000 phase equilibrium data sets. Most of the data were collected along with the experimental uncertainties. Various estimation methods and thermodynamic models were included to calculate properties and phase equilibria. Data can be searched for with a stand-alone program or using an Internet web site. The current status and future prospects of the KDB (Korean Thermophysical Properties Databank) are discussed.

KEY WORDS: database; data bank; data collection; thermophysical properties; vapor–liquid equilibria.

1. INTRODUCTION

Physical properties and phase equilibrium data are the basic information needed for process design and operations. Thermophysical and phase

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equilibrium property data for pure components and mixtures are needed for material and energy balances and for equipment design. A key factor in evaluating process simulation and design programs is the reliability of predicted thermophysical properties and phase equilibria. Such data are usually supplied in various forms. The DDB (Dortmund Data Bank) [1] and DIPPR (Design Institute for Physical Properties) [2] are well-known mixture and pure component physical property databases. It has been recognized that the absence of reliable data and correlations results in a lack of confidence in design calculations [3]. Several authors [3, 4] have reviewed the effect of property estimation errors. In the past, the need for accurate data for comprehensive materials was not a serious problem. With recent advances in process engineering, the need for thermophysical properties and calculation models is growing in Korea. Moreover, with the growing demand for new materials, and environmental and safety considerations, the industry demand for new data and models becomes even greater. With the support of the MOCIE (Ministry of Commerce, Industry and Energy) in Korea, four universities (Korea University, Sogang University, Seoul National University, and KAIST) collaborated to develop a database and experimental measurement capabilities. The main purpose of the KDB (Korea Thermophysical Properties Databank) project is to develop, organize, and maintain useful data compilations and calculation programs.

2. DATA COMPILATION

The database is composed of pure component and mixture property databases and their management system. Components are classified as hydrocarbons, polymers, and electrolytes.

2.1. Pure Component Properties

Entries to the pure component property databank are some 2000 hydrocarbons, 200 polymers, and 2000 electrolytes. Fixed properties collected for each component are as follows.

(a) Hydrocarbons

Basic properties

Molecular weight, critical data, boiling point, freezing point, triple point, acentric factor, solubility parameters, heat of combustion, heat of fusion, partial molar volume, Gibbs free energy, and enthalpy of formation at standard state

Molecular properties

Dipole moment, radius of gyration, Van der Waals volume/area

Point properties

Liquid density, heat of vaporization, surface tension, dielectric constant, refractive index

Hazardous and environmental properties

Flash point, flammability limit, auto ignition temperature, NFPA rating

(b) Polymers

Glass transition temperature, melting point, solubility parameters, dielectric constants, refractive index, surface tension

(c) Electrolytes

Molecular weights, ionic valence, solid density, Gibbs free energy, enthalpy of formation

They are given with values in original units, with references, and with uncertainty information when possible. Raw experimental data for temperature-dependent properties such as vapor pressure, heat capacity, viscosity, thermal conductivity, and surface tension are also given with their regression coefficients.

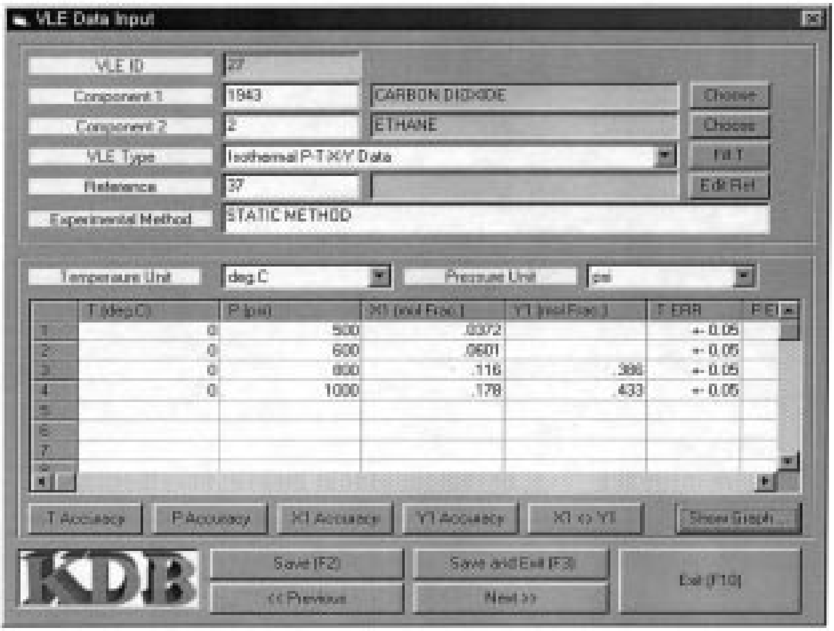
2.2. Mixture Properties

About 5000 sets of phase equilibrium data and mixture properties are provided for hydrocarbon VLE, polymer solubility, and electrolyte solubility. They are provided with references, uncertainty information, and experimental methods. Figure 1 shows a typical binary VLE input program interface.

- Vapor–Liquid equilibrium data (4602 sets)
- Polymer finite solubility (431 sets)
- Polymer infinite solubility (222 sets)
- Aqueous electrolyte solution solubility (501 sets)

2.3. Miscellaneous Data

Atomic weights, dimension conversion table, physical constants, property definition table, and other miscellaneous data tables are also given.



VLE ID: 27
Component 1: 1943 CARBON DIOXIDE
Component 2: 2 ETHANE
VLE Type: Isothermal P-T-X/Y Data
Reference: 37
Experimental Method: STATIC METHOD
Temperature Unit: deg C
Pressure Unit: psi

	T (deg C)	P (psi)	X1 (mol Frac.)	Y1 (mol Frac.)	T ERR
1	0	500	.0372		+- 0.05
2	0	600	.0601		+- 0.05
3	0	800	.116	.386	+- 0.05
4	0	1000	.178	.433	+- 0.05
5					
6					
7					

Fig. 1. Binary VLE experimental data input program of the KDB.

2.4. Databank Management Program

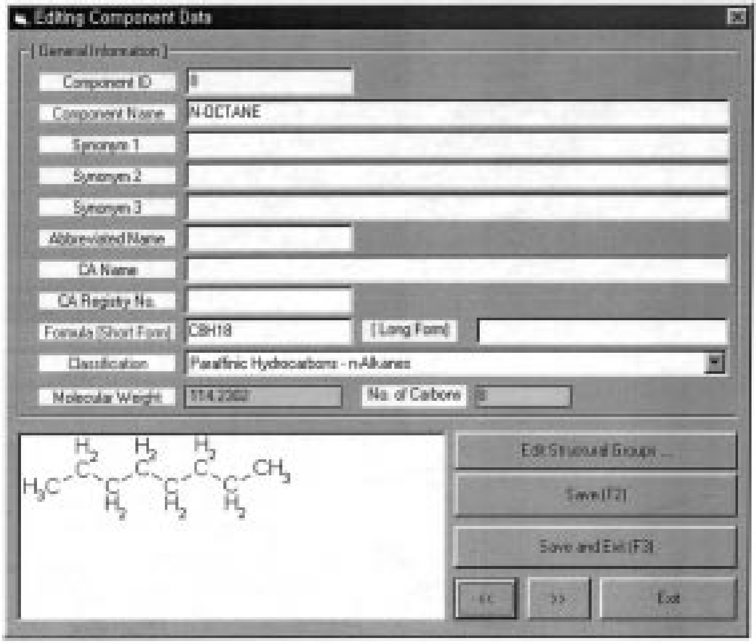
The Databank management program is composed of four parts—data input programs, data verification/regression programs, data transfer programs, and data search/view programs. Working data are stored in local computers and verified data are stored in the DBMS server using Microsoft SQL Server software. Figures 2 and 3 show typical data input programs for hydrocarbon pure component data.

3. CALCULATION MODULES

Calculation modules include FORTRAN 77 source codes for physical property and phase equilibrium calculations. Simple process design programs are also included for testing the thermophysical property calculation modules. The programs available for property calculations are as follows.

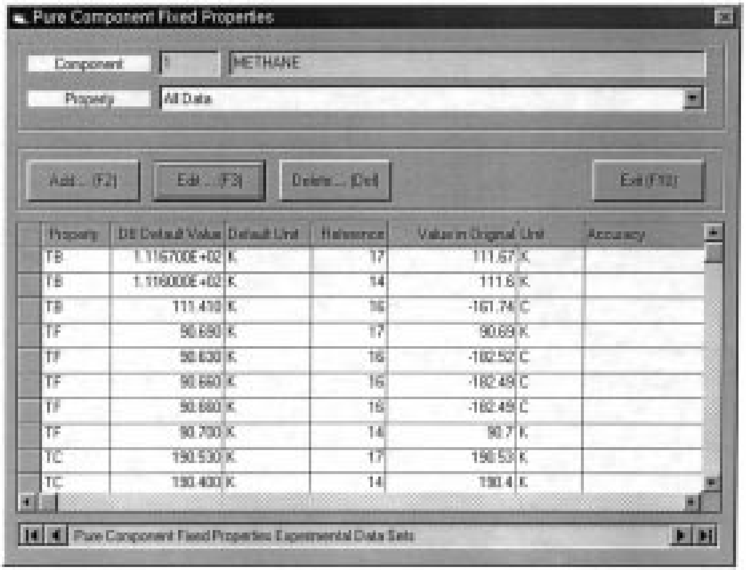
(a) Hydrocarbons

- Vapor pressure calculation, heat of vaporization calculation, gas/liquid density calculation, gas/liquid viscosity calculation,



Component ID	8		
Component Name	N-OCTANE		
Synonym 1			
Synonym 2			
Synonym 3			
Abbreviated Name			
CA Name			
CA Registry No.			
Formula (Short Form)	C8H18	(Long Form)	
Classification	Paraffinic Hydrocarbons - n-Alkanes		
Molecular Weight	114.2302	No. of Carbons	8

Fig. 2. Typical data input program of the KDB.



Component 1 METHANE

Property All Data

Property	DB Default Value	Default Unit	Reference	Value in Original	Unit	Accuracy
TB	1.116700E+02	K	17	111.67	K	
TB	1.116000E+02	K	14	111.6	K	
TB	111.410	K	16	-161.74	C	
TF	90.690	K	17	90.69	K	
TF	90.630	K	16	-182.52	C	
TF	90.660	K	16	-182.49	C	
TF	90.660	K	16	-182.49	C	
TF	90.700	K	14	90.7	K	
TC	190.530	K	17	190.53	K	
TC	190.400	K	14	190.4	K	

Fig. 3. Pure component experimental data input program of the KDB.

  gas/liquid thermal conductivity calculation, gas/liquid heat capacity calculation
- Vapor–liquid equilibrium calculation

(b) Polymers

- Density estimation, glass transition temperature estimation, heat capacity estimation, heat of fusion estimation, cohesive energy estimation, refractive index estimation, solubility parameter estimation
- Polymer solubility calculation

(c) Aqueous electrolyte solutions

- Freezing point lowering calculation, solubility calculation, solution density calculation, solution viscosity calculation, solution vapor pressure calculation,
- Vapor–liquid equilibrium calculation

Essentially, all the property calculation modules for polymer properties are based on group-contribution methods. Models used for equilibrium calculations are as follows.

(a) Hydrocarbon VLE

- Equations of state: SRK EOS (with Wong–Sandler mixing rule) [5], PR EOS (with Wong–Sandler mixing rule) [5], nonrandom lattice fluid model [6, 7]
- Activity models: WILSON model [8], UNIQUAC model [9], UNIFAC model [10]

(b) Polymer solutions

- High–Danner model [11], UNIFAC-free volume model [12], nonrandom lattice fluid model [6, 7]

(c) Aqueous electrolyte solutions

- Pitzer model [12], Chen model [13], Bromley model [14], Meissner model [15], UNIQUAC model [8]

4. EXPERIMENTAL CAPABILITIES

In addition to the effort to collect data in the literature, the four universities in Korea collaborated to enhance their experimental capabilities in their specialized fields. Data production projects were performed in accordance with local industry's demand for specific data.

5. WEB SERVICE

Compiled physical property data and coefficients for calculation modules can be accessed using an Internet web site (http://thermo.korea.ac.kr). WEB service includes the following interface to the databank.

- Unit conversion
- Atomic weights
- Pure component fixed properties
- Temperature-dependent pure properties
- Binary VLE databank
- Polymer solubility databank
- Aqueous electrolyte solution databank

A typical database search result is shown in Fig. 4.

6. FUTURE PROSPECTS

After 3 years of developing the basic structure and collecting literature data, still more effort remains to meet the needs of academia and industry.

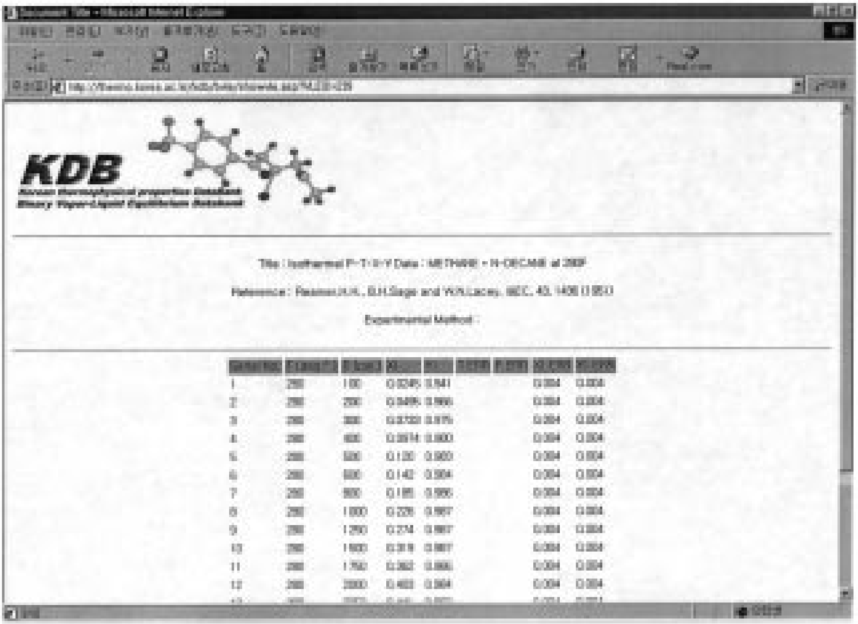


Fig. 4. Internet search result for binary VLE data.

Furthermore, it is estimated that 40–60% of the budget of long-term software is spent on maintenance. With the aid of the KICChE (Korea Information Center for Chemical Engineering), the databank is still growing and its contents are being refined.

7. CONCLUSIONS

The current status of the database project in Korea has been briefly summarized. The project is intended to gather data on specialized fields and construct a database, to enhance experimental capability and produce data, and to develop computational modules for thermophysical properties and equilibria.

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