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PREDICTION OF BINARY AZEOTROPE FORMATION IN HYDROCARBON MIXTURES USING A KNOWLEDGE-BASED EXPERT SYSTEM

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Abstract—In present study, a hierarchical knowledge-based expert system, named HYDROPERT, to predict binary azeotrope formation in hydrocarbon mixtures was created and investigated. Specific knowledge included in azeotropy on hydrocarbon mixtures and the implementation of the expert system are described along some of the several components of expert system applications: knowledge representation strategy and levels of knowledge abstraction, inference machine, user interface, explanation facilities. The knowledge base is hierarchically structured with the multiple levels of domain-specific knowledge such as the azeotropic data bank as the lowest level, component-specific compiled heuristic rules as the second level, group-oriented compiled heuristic rules as the third level, and generic class-oriented model-based heuristic rules as the highest level. The predictive capabilities and generality of the expert system can be highly enhanced through the integration of different kinds of domain knowledge into the hierarchical structure. The expert system predicting the binary azeotrope formation in hydrocarbon mixtures may be a useful tool for many chemical engineering activities, especially such as process synthesis and design.

Key words: *HYDROPERT, Hydrocarbon, Compiled Heuristic, Model-based Heuristic, Binary Azeotrope*

INTRODUCTION

Recently, research in the field of artificial intelligence has had many successful developments. One of the most significant areas of artificial intelligence is the development of powerful new computer systems known as "knowledge-based" expert systems [Stephanopoulos and Mavrovouniotis, 1988]. The considerable development of knowledge-based expert systems could afford the use of expert system as a practical auxiliary tool in the field of chemical engineering [Banares et al., 1988]. Until now, in the field of chemical engineering the process synthesis and fault diagnosis using knowledge-based expert systems have been actively researched [Simmrock et al., 1990].

In the case of process synthesis expert systems are used to determine the best sequencing of columns in the most efficient way with heuristic rules. Most of the process synthesis studies in the field of separation have been concerned with multicomponent ideal mixtures, because there is no difficulty in predicting which components can be made to come off the top of a column and which can be made to come off the bottom. However, this process synthesis may be highly complicated by forming of azeotropes due to nonidealities in mixtures. These azeotropes can make a given separation impossible by ordinary distillation and the mixture must be separated by using the special separation processes such as azeotropic distillation or extractive distillation. An information of occurrence of azeotropes in the mixture is thus one of the basic and most important thermodynamic data to produce a judicious design for the separation step. Furthermore, an understanding of azeotropes is also important for the selection of successful entrainers in azeotropic distillation, for the selection of auxiliary materials in extractive distillation and for the selection of proper solvents in extraction.

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First of all, expert systems can be used in the area having no exact theories for problem solving. Therefore, it would be desirable to develop an expert system for the efficient prediction of the occurrence of binary azeotropes in hydrocarbon mixtures by formulating a chunk of informations on azeotropy that have been reported until now in form of theories and experimental data into the heuristic rules and important to chemists and chemical engineers in the synthesis, design, and operation of chemical processes.

In order to predict an occurrence of binary azeotropes in hydrocarbon mixtures, a hierarchical knowledge-based expert system has been constructed. Domain-specific knowledge on azeotropy is hierarchically implemented with the aid of the declarative programming language Prolog [Böhringer et al., 1988] into several different knowledge levels such as the more specific COMPONENT level, GROUP level, and the generic model-based CLASS level. Further, the expert system has been linked to an azeotrope data bank in order to determine whether or not experimental data is already available. In this article, basic theories on azeotropy and some functions of the expert system for the prediction of the occurrence of binary azeotropes in hydrocarbon mixtures, will be discussed. First, it will be given a general review of theoretical basis on azeotropy. Next, the architecture of the expert system will be presented, showing knowledge abstraction and representation, the problem-solving strategy and system implementation for predicting binary azeotrope formation in hydrocarbon mixtures based on heuristic knowledge.

AZEOTROPY

Azeotrope means literally that the vapor boiling from a liquid has the same composition as the liquid [Kurtyka, 1988]. An azeotrope exhibits a minimum or maximum boiling point at an azeotrope point according to the Gibbs-Konovalov theorem [Konova-

lov, 1881]. This theorem is a practically important condition in chemical engineering, especially in the area of process design and synthesis, because it limits the possibility of separation by common fractional distillation. Whether or not a binary mixture is azeotropic depends essentially upon following two factors:

—the degree of nonideality of a mixture

—the difference in boiling points between two pure components.

The nonideality of the mixture depends largely on the intermolecular forces of the components such as dispersion forces, dipole-dipole interactions, dipole-induced dipole interactions, and hydrogen bonding, of which latter is the most important effect on azeotrope formation. The closer the boiling points of the two components are, the more likely they will be azeotropic; the more ideal the solution of the two components is, the less likely they will form an azeotropic system [Horsley, 1973].

Until now a number of workers have proposed several independent correlations [Edan et al., 1980] to predict binary azeotrope formation in hydrocarbon mixtures with the thermodynamic properties of mixtures in the practical side. However, they are highly empirical and specific. It appears difficult to find out the physical basis, which is able to generally apply to all kinds of hydrocarbon mixtures, because the theoretical aspects of azeotropy, especially of intermolecular forces is little developed.

A more general and accurate prediction of azeotrope formation can be achieved by taking account of the classification of hydrocarbon mixtures based on the series of homologues (alkanes, alkenes, aromatics, etc.) appearing the similar degree of nonideality and the difference in boiling points between the two pure components without the accurate informations of intermolecular forces. Boiling point difference effect on azeotropy can be well explained with the "azeotropic range" concept that was introduced by Swietoslawski [1950] and has been developed by Malesinki [1956] and Yoshimoto [1956] on the general assumption that the components form a regular solution. These concepts may be successfully and efficiently used for the prediction of binary azeotrope formation in hydrocarbon mixtures with an expert system because of the generality of the concepts, the small number of parameters, and the simplicity of parameters.

1. The Series of Azeotropes and Azeotropic Range

The most useful characteristics of azeotropes is the azeotropic range defined by Swietoslawski and developed by Yoshimoto and Malesinski on the general assumption that the components form a regular solution. The azeotropic range concept has played an important role in the area of azeotropy and has been used by many workers in recent studies [Kurtyka, 1975] to predict azeotrope formation in mixtures. The azeotropic range can be defined as follows [Malesinski, 1956].

The azeotropic range can be considered as the maximum pure component boiling point difference within which azeotropes formed by a certain component 1 with successive homologues 2i; only mixtures formed with homologues boiling within a certain temperature range (T_{2l}, T_{2u}) below and above the boiling temperature T_1 of a component 1 exhibit minimum azeotropes. That is the range of formation of azeotropes is limited by two characteristics, azeotropes (1, 2u) and (1, 2l), having respectively the compositions $x_1=1.0$ and $x_1=0$ and boiling temperature T_1 and T_{2l} respectively. These limiting azeotropes are called the upper tangent azeotrope and the lower tangent azeotrope. The difference in the boiling temperatures of the homologues forming the tangent azeotropes is called the azeotropic range Z:

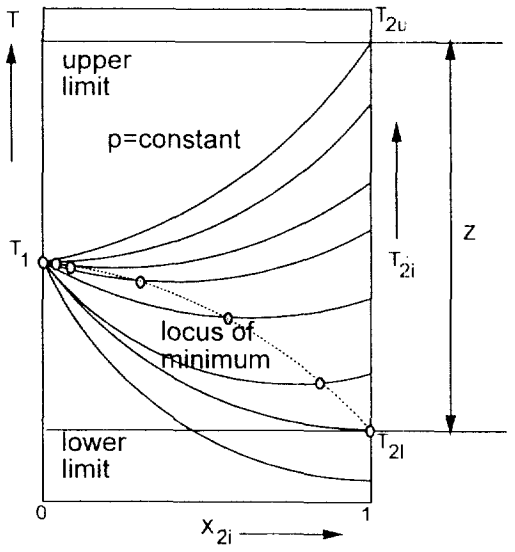

Fig. 1. The azeotropic range of binary azeotropes.

$$Z=T_{2u}-T_{2l}.$$

Without this azeotropic range concept, some general conditions for predicting azeotrope formation could not be formulated. Thus, the component classification based on the series of homologues and the azeotropic range can be the underlying concepts to predict binary azeotrope formation in hydrocarbon mixtures with reasonable accuracy.

KNOWLEDGE ABSTRACTION

1. Binary Azeotropic Data Bank

The binary azeotropic data bank mainly contains experimental binary azeotropic data taken from the Horsley's Azeotropic Data Book [1973] and it has been complemented by our own comprehensive collection of experimental binary azeotropic data published in the literature since 1972. No attempt has been made to evaluate the accuracy of the azeotropic data. At present 18502 binary azeotropic data sets including hydrocarbon systems are stored in the binary azeotropic data bank.

The compiled heuristic rules used in HYDROPERT for the prediction of binary azeotrope formation in hydrocarbon systems have been formulated within this contribution on the basis of the azeoptropic ranges between the series of hydrocarbon homologues that have been estimated by the case studies with the modified azeotropic data bank. The modified azeotropic data bank was created by connecting the binary azeotropic data bank and another data bank including components and their corresponding homologue names for group identification. All the data banks 3in this work was implemented with the Foxbase data base system.

The structure of the data bank for group identification is shown in Fig. 2. This data bank includes the homologous names of all hydrocarbons which are stored in the binary azeotropic data bank. Fig. 2 shows the structure of the modified azeotropic data bank. Each data record contains formulas, component names, the occurrence of binary azeotrope, group names, system pressure, azeotrope temperature, normal boiling points, and the difference of the normal boiling points.

The query window for the modified azeotropic data bank was programmed with the Foxbase data base language. All group-ori-

Formula	Name	Formula	Name		Group	Group	Press. (Mpa)	T_a [°C]	T_1 [°C]	T_2 [°C]	ΔT [°C]
C8H18	OCTANE	C6H6	BENZENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	125.75	80.10	-45.65
C7H16	HEPTANE	C6H6	BENZENE	AZE	N-ALKANE	AROMATIC	0.10130	80.100	98.40	80.10	-18.30
C8H18	OCTANE	C7H8	TOLUENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	125.75	110.70	-15.05
C9H20	NONANE	C8H10	ETHYL BENZENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	150.70	136.15	-14.55
C9H20	NONANE	C8H10	P-XYLENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	150.70	138.40	-12.30
C9H20	NONANE	C8H10	O-XYLENE	AZE	N-ALKANE	AROMATIC	0.10130	144.250	150.70	143.60	-7.10
C9H20	NONANE	C8H8	STYRENE	AZE	N-ALKANE	AROMATIC	0.10130	144.000	150.70	145.00	-5.70
C9H20	NONANE	C9H12	CUMENE	AZE	N-ALKANE	AROMATIC	0.10130	148.000	150.70	152.80	2.10
C8H18	OCTANE	C8H10	ETHYL BENZENE	AZE	N-ALKANE	AROMATIC	0.10130	125.600	125.75	136.15	10.40
C6H14	HEXANE	C6H6	BENZENE	AZE	N-ALKANE	AROMATIC	0.10130	68.500	68.95	80.10	11.15
C7H16	HEPTANE	C7H8	TOLUENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	98.40	110.70	12.30
C8H18	OCTANE	C8H10	P-XYLENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	125.75	138.40	12.65
C7H16	HEPTANE	C8H10	ETHYL BENZENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	98.40	136.15	37.75
C7H16	HEPTANE	C8H10	P-XYLENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	98.40	138.40	40.00
C6H14	HEXANE	C7H8	TOLUENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	68.95	110.70	41.75
C5H12	PENTANE	C6H6	BENZENE	NON	N-ALKANE	AROMATIC	0.10130	0.000	36.15	80.10	43.95

T_a : azeotrope temperature
T_1 : normal boiling point of component 1
T_2 : normal boiling point of component 2
ΔT : the difference of the normal boiling points ($T_2 - T_1$)
AZE : binary azeotrope
NON : nonazeotrope

Fig. 2. The structure of the data bank derived from the case study for system n-alkane/aromatic.

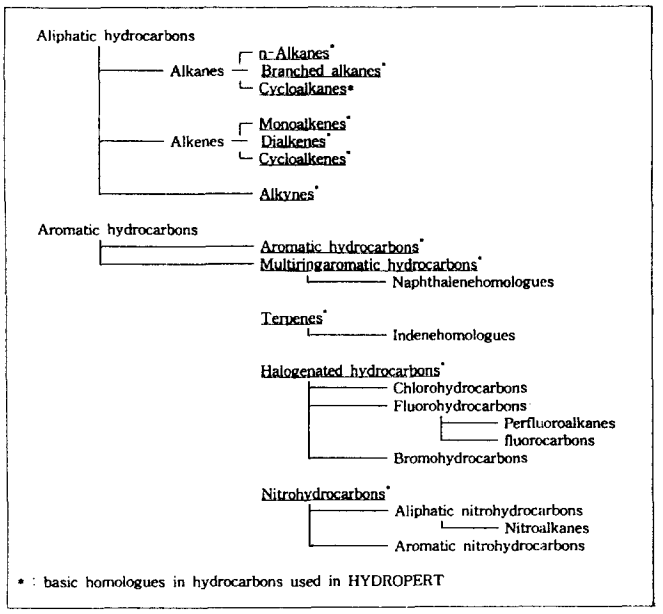

Fig. 3. Taxonomy of hydrocarbons used in knowledge abstraction.

Component A		Component B		Group A	Group B		ΔT[℃]
C8H18	OCTANE	C6H6	BENZENE	N-ALKANE	AROMATIC	NON	-45.65
C7H16	HEPTANE	C6H6	BENZENE	N-ALKANE	AROMATIC	NON	-18.30
C8H18	OCTANE	C7H8	TOLUENE	N-ALKANE	AROMATIC	NON	-15.05
C9H20	NONANE	C8H10	ETHYL BENZENE	N-ALKANE	AROMATIC	NON	-14.55
C9H20	NONANE	C8H10	P-XYLENE	N-ALKANE	AROMATIC	NON	-12.30
C9H20	NONANE	C8H10	O-XYLENE	N-ALKANE	AROMATIC	AZE	-7.10
C9H20	NONANE	C8H8	STYRENE	N-ALKANE	AROMATIC	AZE	-5.70
C9H20	NONANE	C9H12	CUMENE	N-ALKANE	AROMATIC	AZE	2.10
C8H18	OCTANE	C8H10	ETHYL BENZENE	N-ALKANE	AROMATIC	AZE	10.40
C6H14	HEXANE	C6H6	BENZENE	N-ALKANE	AROMATIC	AZE	11.15
C7H16	HEPTANE	C7H8	TOLUENE	N-ALKANE	AROMATIC	NON	12.30
C8H18	OCTANE	C8H10	P-XYLENE	N-ALKANE	AROMATIC	NON	12.65
C7H16	HEPTANE	C8H10	ETHYL BENZENE	N-ALKANE	AROMATIC	NON	37.75
C7H16	HEPTANE	C8H10	P-XYLENE	N-ALKANE	AROMATIC	NON	40.00
C6H14	HEXANE	C7H8	TOLUENE	N-ALKANE	AROMATIC	NON	41.75
C5H12	PENTANE	C6H6	BENZENE	N-ALKANE	AROMATIC	NON	43.95

NON: nonazeotrope AZE: azeotrope $\Delta T[℃]$: $T_{aromatic} - T_{n\text{-}alkane}$

Fig. 4. The azeotropic range for n-alkanes and aromatics.
($\Delta T = T_{aromatic} - T_{n\text{-}alkane}$, T = normal boiling point)

ented compiled heuristic rules in HYDROPERT were formulated by the case studies performed with this query window. For example, the heuristic rules for the system n-alkane/aromatic can be formulated as follows: Firstly, the group names, n-alkanes and aromatics, are inputted through the query window. Then, the data bank, which contains all binary data for the system n-alkane/aromatic, extracted from the modified binary azeotropic data bank, is created. Based on this data bank, the heuristic rules for the system n-alkane/aromatic are formulated.

2. Heuristic Rules for the Prediction of Binary Azeotrope Formation in Hydrocarbons

In order to perform the case studies with the azeotropic data bank all hydrocarbons have been divided into 12 basic homologues. And in some cases, these basic homologues have been further divided into subgroups in order to specialize the heuristic rules when the members of a certain subgroup show an exceptional azeotropic range. Fig. 3 shows the basic homologues in hydrocarbons and a taxonomy of hydrocarbon compounds used in order to carry out the case studies.

The reason behind this approach is that while the members of a homologous series form essentially ideal solutions, they form

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Rule : Group 8

Two components K1 and K2 form an azeotrope,
    if component K1 belongs to the n-alkanes
      and if component K2 belongs to the aromatic hydrocarbons
      and if T1[℃] is the normal boiling point of component K1
      and if T2[℃] is the normal boiling point of component K2
      and if the difference between the boiling points(T2-T1) is >= -8.0
      and if the difference between the boiling points(T2-T1) is =< 12.0.

Rule : Group 8.1

Two components K1 and K2 do not form an azeotrope,
    if component K1 belongs to the n-alkanes
      and if component K2 belongs to the aromatic hydrocarbons
      and if T1[℃] is the normal boiling point of component K1
      and if T2[℃] is the normal boiling point of component K2
      and if the difference between the boiling points(T2-T1) is =< -14.5
          or the difference between the boiling points(T2-T1) is > 12.0.
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Fig. 5. The group-oriented heuristics for n-alkanes and aromatics.

more nonideal solutions with another component in different homologues. That is, the nonideality of a mixture can be explained in terms of the combination of the different series of homologues. The result of case studies indicates that azeotrope formation can be good predicted with the azeotropic ranges between the series of homologues formulated by theoretical considerations.

As shown in Fig. 4, the azeotropic range contains two limits: the lower and the upper boundary in which an azeotrope will be formed. The boundary values of each group-oriented compiled heuristic rule were adopted from the tables derived by the case study like Fig. 4. Based on these tables, when each heuristic rule was formulated, the lower and the upper boundary values were strictly interpreted for the accuracy of prediction.

For example, the rule Group_8 shown in Fig. 5 can be formulated from Fig. 4. Fig. 5 shows that the lower boundary of the azeotropic range for the system aromatic/n-alkane is located between -12.30 and -7.10 and the upper boundary of the azeotropic range is located between 11.15 and 12.30. Although as the azeotropic range one can adopt a middle value -9.7 for the lower boundary and 11.73 for the upper boundary, high certainty region with reasonable tolerance (between -8.0 and 12.0) is adopted as the azeotropic range for the accuracy of prediction. In practice, it is reasonable to give some tolerance for the difference of normal boiling points because there are very frequently different normal boiling point data for the same component in the literature. The boundary values of the nonazeotropic region are also strictly interpreted as shown in Fig. 5. The occurrence of binary azeotropes in the uncertainty regions, between -14.5 and -8.0 for the lower region, may be qualitatively predicted with model-based heuristics used as default reasoning in HYDROPERT.

Fig. 6 shows some group-oriented compiled heuristic rules implemented in the knowledge base of HYDROPERT. These rules do not explicitly use the specific component and hence they can be used to generally predict binary azeotrope formation regardless of the specific hydrocarbon components. Fig. 7 represents a component-specific compiled heuristic rule which is mainly concerned with the tendency of binary azeotrope formation between a certain hydrocarbon component and a series of hydrocarbon homologues. These types of heuristic rules are characterized by less generality and high degree of accuracy due to their component-specific characteristics. The component-specific heuristic rules can be considered as the more specialization of group-oriented heuristics. These rules have been mostly formulated on the basis of research results published in the literature because it is impossible to carry out the case studies with the azeotropic data bank due to a great number of components in hydrocarbons. Through our own case studies based on the experimental binary hydrocarbon azeotropic data in the azeotropic data bank and research results published in the literature, total about 70 positive and negative compiled heuristics were derived and implemented into the knowledge base of HYDROPERT. According to our experience, predictions with these compiled heuristic rules as to whether a given hydrocarbon mixture be a binary azeotrope or not were successful at more than 95% probability.

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Rule : Group 1

Two components K1 and K2 do not form an azeotrope,
  if component K1 belongs to the n-alkanes
     and if component K2 belongs to the n-alkanes.

Rule : Group 2

Two components K1 and K2 form an azeotrope,
  if component K1 belongs to the n-alkanes
     and if component K2 belongs to the branched alkanes
     and if T1[℃] is the normal boiling point of component K1
     and if T2[℃] is the normal boiling point of component K2
     and if the difference between the boiling points(T2-T1) is >= -1.0
     and if the difference between the boiling points(T2-T1) is =< 1.0.

Rule : Group 3

Two components K1 and K2 form an azeotrope,
  if component K1 belongs to the n-alkanes
     and if component K2 belongs to the cycloalkanes
     and if T1[℃] is the normal boiling point of component K1
     and if T2[℃] is the normal boiling point of component K2
     and if the difference between the boiling points(T2-T1) is >= 0.0
     and if the difference between the boiling points(T2-T1) is =< 4.0.

Rule : Group 3.1

Two components K1 and K2 do not form an azeotrope,
  if component K1 belongs to the n-alkanes
     and if component K2 belongs to the cycloalkanes
     and if T1[℃] is the normal boiling point of component K1
     and if T2[℃] is the normal boiling point of component K2
     and if the difference between the boiling points(T2-T1) is =< -4.0
         or the difference between the boiling points(T2-T1) is > 4.0.

Rule : Group 4

Two components K1 and K2 form an azeotrope,
  if component K1 belongs to the n-alkanes
     and if component K2 belongs to the monoalkenes
     and if T1[℃] is the normal boiling point of component K1
     and if T2[℃] is the normal boiling point of component K2
     and if the difference between the boiling points(T2-T1) is >= 0.0
     and if the difference between the boiling points(T2-T1) is =< 2.0.

Rule : Group 4.1

Two components K1 and K2 do not form an azeotrope,
  if component K1 belongs to the n-alkanes
     and if component K2 belongs to the monoalkenes
     and if T1[℃] is the normal boiling point of component K1
     and if T2[℃] is the normal boiling point of component K2
     and if the difference between the boiling points(T2-T1) is =< -3.0
         or the difference between the boiling points(T2-T1) is > 2.0.
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Fig. 6. Some examples of compiled heuristic rules implemented in the knowledge base.

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Rule : Aromatic-1

Two components K1 and K2 form an azeotrope,
    if component K1 is benzene
      and if component K2 belongs to the n-alkanes
      and if the normal boiling point of component K2 is >=68.0 ℃
      and if the normal boiling point of component K2 is =<100.0 ℃
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Fig. 7. The component-oriented heuristic for benzene and n-alkanes.

The model-based heuristics for the prediction of binary azeotrope formation in hydrocarbon mixtures have been developed on the basis of Eduljee and Tiwari's work [1976]. Eduljee and Tiwari have proposed a correlation that shows the azeotropic range within which azeotropes formation is possible, based on

Rule : Class_9

Two components K1 and K2 probably form an azeotrope,
if component K1 belongs to the class 1
and if component K2 belongs to the class 3
and if T1[℃] is the normal boiling point of component K1
and if T2[℃] is the normal boiling point of component K2
and if the difference of the normal boiling points(T2-T1) is ≥ -26.0 ℃
and if the difference of the normal boiling points(T2-T1) is ≤ 27.0 ℃.

Rule : Class_9.1

Two components K1 and K2 do not probably form an azeotrope,
if component K1 belongs to the class 1
and if component K2 belongs to the class 3
and if T1[℃] is the normal boiling point of component K1
and if T2[℃] is the normal boiling point of component K2
and if the difference of the normal boiling points(T2-T1) is < -26.0 ℃
or the difference of the normal boiling points(T2-T1) is > 27.0 ℃.

Fig. 8. Model-based heuristic rules.

Yoshimoto's correlation [1956] developed from regular solution theory and a classification which groups organic compounds according to their hydrogen bonding characteristics. Total 13 positive and 13 negative model-based heuristics [Eduljee and Tiwari, 1976] were implemented in the knowledge base and typical model-based heuristics are shown in Fig. 8. In HYDROPERT they are considered as a default reasoning method which is finally used, when the compiled reasoning fails to make a reasoning due to their more generic and less accurate characterstics.

PROBLEM-SOLVING STRATEGY AND IMPLEMENTATION

The problem-solving strategy of HYDROPERT is quite different from that of conventional predictive expert systems. Many conventional expert systems use only compiled knowledge in order to draw a reasoning. HYDROPERT makes use of several different problem-solving methods such as component-specific, group-oriented, and model-based heuristic reasoning. Each problem-solving method can be invoked sequentially or separately until making a reasoning. The problem-solving strategy of HYDROPERT is summarized in Fig. 9.

The problem-solving procedure of HYDROPERT is carried out as follows: HYDROPERT first examines the binary azeotropic data bank, in order to confirm whether there are already the azeotropic data for the consulted binary hydrocarbon system. If there are no azeotropic data for the consulted binary system, HYDROPERT automatically invokes its component-specific knowledge base to draw reasoning on the basis of the facts about the consulted binary system. If there are no component-specific heuristics in the knowledge base that apply to the consulted binary system, the reasoning will automatically proceed on to the next level, the group-oriented heuristics. In most cases, the occurrence of an azeotrope in a binary hydrocarbon system can be predicted with these group-oriented compiled heuristics. However, if this reasoning method fails too, finally, HYDROPERT can qualitatively predict binary azeotrope formation with the model-based heuristic reasoning that can be regarded as a default reasoning method. In this manner, HYDROPERT can effectively and reliably predict binary azeotrope formation in a wide variety of hydrocarbon systems regardless of known or unknown azeotropic systems.

As shown in Fig. 10, the structure of the knowledge-based ex-

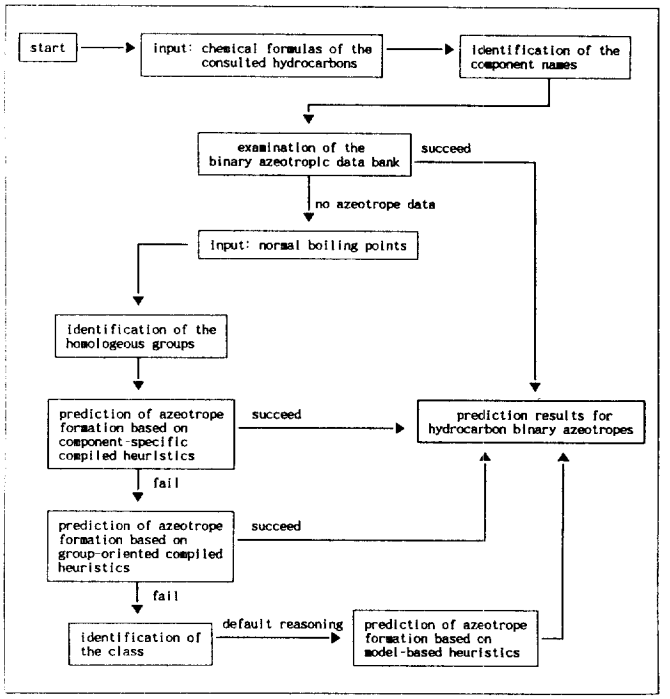

Fig. 9. Problem-solving strategy of HYDROPERT.

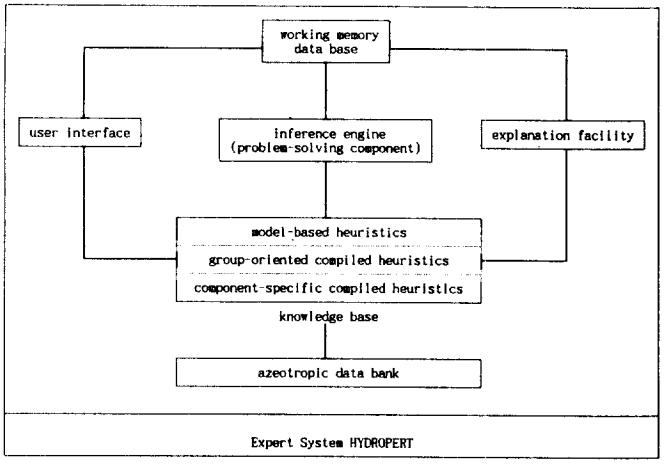

Fig. 10. Architecture of HYDROPERT.

pert system HYDROPERT is largely divided into the user interface to provide the required data and to interact with the user, a working memory data base where data about the problem are stored temporarily as facts, the knowledge base in which different kinds of domain-specific knowledge are hierarchically encoded, an inference engine that makes a predictive reasoning, and finally, the explanation facilities to help users during a predictive consultation. Moreover, HYDROPERT is connected with an azeotropic data bank including the binary azeotropic data and the azeotropic data bank can be considered as the lowest level of the knowledge base.

The whole computing environment of HYDROPERT was programmed in IF/PROLOG artificial intelligence programming language, which is a Prolog dialect of the Edinburgh syntax. It offers significant advantages in applications whose nature entails symbolic computation rather than numerical operations and is thus

a suitable programming language for HYDROPERT implementation because most of operations in HYDROPERT are concerned with symbolic manipulation.

CONCLUSIONS

The knowledge-based expert system HYDROPERT for the prediction of binary azeotrope formation in a hydrocarbon mixture discussed in this study may be an intelligent aid to chemical engineers, especially in the area of process synthesis. The domain-specific knowledge on azeotropy for hydrocarbon mixtures has been implemented in the knowledge base of HYDROPERT using a hierarchically structured, flexible and reliable knowledge representation. The architecture demonstrated here in HYDROPERT may successfully contribute to the prediction of binary azeotrope formation in a wide variety of hydrocarbon mixtures. This hierarchical approach using the different types of knowledge makes the problem-solving method of HYDROPERT more powerful and flexible and is a more natural model of a human reasoning process.

HYDROPERT flexibly makes a reasoning with the integration of compiled knowledge derived from the generalization of a large number of case studies with the azeotropic data bank and model-based knowledge derived from deep knowledge, the regular solution theory. The explanation facility of HYDROPERT makes it possible to follow the predictive reasoning procedures, thus fulfilling the reasoning transparency requirement. When HYDROPERT makes a conclusion, it explains how a reasoning was made.

The following important issues have been treated and achieved to a large degree in this research; multiple levels of knowledge abstraction, hybridity of problem-solving methodology, modularity of programming, the integration of a data bank into the knowledge base. In particular, experience in implementation of HYDROPERT has shown that it is necessary to make use of hybrid systems in several aspects such as knowledge representation and abstraction, problem-solving strategies, etc.

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NOMENCLATURE

T_i : normal boiling point of component i [℃]
T_{2i} : normal boiling point of a series of homologues at binary systems [℃]
T_{az} : azeotrope temperature [℃]
T_{2l} : lower tangent azeotrope temperature [℃]
T_{2u} : upper tangent azeotrope temperature [℃]
x_i : mole fraction of component i at binary systems
X_{2i} : mole fractions of a series of homologues at binary systems
Z : azeotropic range [℃]

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