Computer-Assisted Thermal Analysis System Founded on Case-Based Reasoning

Takashi Nakayama* and Koichi Tanaka

Department of Information Sciences, Faculty of Science, Kanagawa University, 2946 Tsuchiya, Hiratsuka-shi, Kanagawa, Japan 259-1294

Yuko Nishimoto

Department of Materials Sciences, Faculty of Science, Kanagawa University, 2946 Tsuchiya, Hiratsuka-shi, Kanagawa, Japan 259-1294

Received November 16, 1998

A prototype system which supports thermal analysis by reasoning measurement conditions for a given sample material is described. The process of thermal analysis consists of three steps: (1) set-up measurement conditions; (2) take measurements; and (3) analyze the measurement result. The system supports the first step of the process, which is implemented as a kind of expert system founded on case-based reasoning, giving a solution to a new problem by retrieving a similar past case solved successfully and by modifying the case to fit the problem. A case of thermal analysis is represented from the two points of view, that is, (1) sample information as a material and (2) the purpose of measurement, and the similarity between cases is defined from the two viewpoints accordingly. Case-based reasoning is employed as a reasoning framework for this problem, since the information of measurement conditions is not provided as well-formed structures and is hard to arrange.

1. INTRODUCTION

Thermal analysis, a useful analysis method which measures the thermal characteristics of materials irrespective of their form or state, is increasingly being used in various fields.[1−3] The process of thermal analysis is divided into three steps: (1) set-up of measurement conditions; (2) measurement; and (3) analysis of the measurement result. While the second and third steps are controlled and assisted by computers, the first step is carried out manually on the basis of empirical knowledge and information. The reason for the difficulty in simple computerization stems from an insufficient collection and arrangement of data and knowledge of the measurement conditions of thermal analysis. This situation troubles nonexperts of thermal analysis when measuring their problems. TASC (computer-assisted thermal analysis system), the system described in this paper, is an expert system which carries out the set-up of measurement conditions based on CBR (case-based reasoning).[4−7] The reasoning framework of CBR is between MBR (memory-based reasoning), which solves problems using a large number of specific data, and RBR (rule-based reasoning), which uses a relatively small number of general rules.[8−11] Since an algorithmic method for setting up measurement conditions of thermal analysis is not known so far, some kind of knowledge processing system is required for solving the problem. If RBR is employed as a reasoning mechanism, the condition-parts of rules do not match with most actual problems. On the other hand, the amount of specific data for thermal analysis is not sufficient to apply MBR to this problem. Therefore, it seems suitable to employ CBR as a reasoning framework for the problem of setting up measurement conditions of thermal analysis. Solving problems by using experiences from previous cases in new situations seems to be common to human experts, who often give a solution by recalling their experience of measurement, selecting similar cases, and modifying them on the basis of their knowledge, consulting books and databases if necessary. The system has a collection of past cases of thermal analysis containing actual measurement conditions (i.e., the case base) and related information, and it solves a new problem by retrieving a similar case in the case base and modifying it appropriately so that it fits the problem under study. Whether the proposed measurement condition really works needs to be ascertained by actual measurement. If the measurement succeeds, it will be added to the case base. In order to modify a past case to adapt a new problem, various data, knowledge, and procedures are needed. All of these ought to be the components of a CBR system. Thus, TASC can be viewed as an integrated system of various modules, which treats DTA (differential thermal analysis) and DSC (differential scanning caliometry) as a thermal analysis method and assumes polymeric materials as major measurement objects.[12−14] TASC consists of common CBR modules, such as the case base, problem analyzer, case retriever, case modifier, and several knowledge bases,[6,8] which have the following features:

(1) The case of thermal analysis is represented from two points of view, sample information as a material and measurement purpose, which give the bases for setting up measurement conditions.

(2) The similarity of thermal analysis cases is defined on the basis of the two viewpoints above.

(3) A classification tree, a thesaurus, and a concept dictionary—in other words, an ontology—are provided to enable flexible treatment of terms used for representing and retrieving cases.

10.1021/ci980160i CCC: $18.00
Published on Web 07/23/1999

Table 1. Terms for Thermal Characteristics

	basic	industrial
physical	glass transition, crystallization, melting, crystal-crystal transition, deformation mechanism, entropy, enthalpy, specific heat, heat transfer, thermal diffusion, phase equilibrium, dissolution, surface, viscosity, stabilization mechanism	softening, fluidity, solidity, extensibility, aging, thermal expansion, thermal stress, thermal deformation, heat treatment, insulating
chemical	thermosetting, thermopolymerization, photopolymerization, thermal decomposition	gel, heat resistance, incombutiblity, durability

[a] The terms are categorized roughly such that basic and physical properties are located at left and top area, and industrial and chemical properties are located at right and bottom area of the table, although the categorization is not rigid.

(4) Rule bases are provided to perform case modification or adaptation, and the rules are classified hierarchically according to the degree of generalization of descriptions, giving variations of case modification.

2. CASE REPRESENTATION OF THERMAL ANALYSIS

The case of thermal analysis consists of the following components: (1) the purpose of measuring a sample (measurement purpose), (2) information about the material to be measured (sample information), (3) measurement conditions, (4) the results of measurement, and (5) bibliographical items.

2.1. Measurement Purpose. The measurement purpose of thermal analysis can be described in two ways: in terms of application or in terms of thermal characteristics. Hereafter, the two purposes are referred to as A-purpose and C-purpose, respectively.

(1) A-Purpose. An application purpose is expressed by a sentence written in English, which typically appears as the title of a measurement report. It can be viewed as an interpretation of the characteristics of a sample from a concrete or a general standpoint of an application. Examples are “The estimation of thermal expansion of floppy disks”, “Phase diagram of polymer blend”.

(2) C-Purpose. This is expressed by a list of thermal characteristics to be measured, which can be interpreted as a measurement purpose, since the peaks and shifts in the spectrum obtained as a result of a measurement correspond immediately to thermal characteristics such as glass transition, crystallization, melting. For instance, terms relating to thermal characteristics of polymeric materials are listed in Table 1.[15] The expression of C-purpose gives a model of measurement purpose in terms of attribute values (thermal characteristics) which is equivalent with the A-purpose. In other words, it is an expression of a sentence in terms of lower level descriptions, that is, an expression in the thermal characteristic space. For instance, an A-purpose Phase diagram of polymer blend is converted to the C-purpose list (glass transition, melting).

2.2. Sample Information. The sample information of a measurement case is described by the following items.

(1) Sample Names. The name of a sample is given in any nomenclature including formal names, trivial names, product names, or abbreviations. A thesaurus is provided to assure the uniqueness of various nomenclatures, in which synonyms and related terms are registered, giving flexibility to the retrieval and building the case base. However, a sample name is not an essential item of a case.

(2) Class Names. Samples can be classified from various viewpoints and standards, and they can therefore be identified not only specifically but also by the general categories (i.e., class names) they belong to. For instance, the class name “polymer blend” is given to specific samples like polystyrene, poly-2-chlorostyrene, and so forth. Samples belonging to the same class are considered similar materials from the point of view of the classification. (Conversely, the classification standard is set so that a group of similar samples makes a class.) A decision tree whose nodes are the class names is supplied to decide the category of a given sample. The decision tree is called a classification tree here. As *is-a* relations hold between the nodes linked directly on the tree, *is-a* reasoning can be performed on the classification tree. A class name is essential for any sample to be specified. On the other hand, a class name is also an item of the concept dictionary explained later, and items of the concept dictionary other than class name can therefore be accessed from the class name.

(3) Constitution. If a sample consists of several materials, its constitution is described as follows:

constitutingRelation (material-1, material-2, ...).

For example, the following constitution expresses that a sample is made up of a blend of polystyrene and poly-2-chlorostyrene:

blend (polystyrene, poly-2-chlorostyrene)

(4) Production Process. Usually, a sample is obtained through several steps of a production process. Each step of the production process is described as a list below, and the overall production process is represented as a list of these element lists.

(startingMaterial, product, processingMethod,
temperature, duration)

The product of a given step is identical with the starting material of the next step, and the product of a final step thus becomes a sample. For instance, if the following is the production process of a polymer blend of polystyrene and poly-2-chlorostyrene

“The blended sample was obtained by precipitating a
benzene solution of a mixture of polystyrene and
poly-2-chlorostyrene into methanol and then
pressing the product to make uniform film”

then following two lists would describe the process

((polystyrene, poly-2-chlorostyrene),
polystyrene | poly-2-chlorostyrene, precipitate
(benzeneSolution, methanol), nil, nil)

((polystyrene | poly-2-chlorostyrene),
polystyrene | poly-2-chlorostyrene, press
(polystyrene | poly-2-chlorostyrene), nil, nil)

where the processing methods are expressed in the form of predicates.

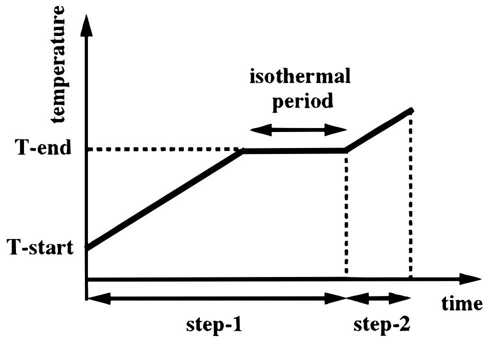

Figure 1. A prototypical example of a temperature program is shown, which controls the overall heating process during the measurement. The unit of a program is called a step, which is specified by four parameters: start temperature, end temperature, heating rate and retention time. A temperature program consists of several consecutive steps specified by those parameters. T-start and T-end in the figure indicate the starting and end temperature of heating in the first step (step 1).

(5) Form. The form of a sample which could effect the result of measurement is described. Examples are lamina, film, and grain.

2.3. Measurement Conditions. Measurement conditions of thermal analysis are described by the following items.

(1) Measuring Device. DSC (differential scanning calorimetry) or DTA (differential thermal analysis) is selected according to the purpose of the measurement. The device actually used is described in a case.

(2) Temperature Program. It is the program which controls the heating process. The program is a combination of one or more steps, each of which is specified by four parameters: start temperature, end temperature, heating rate, and isothermal period. A typical diagram of a temperature program is shown in Figure 1.

(3) Purde Gas. The kind and flow of purde gas that fills the surroundings of the sample and the device are described.

(4) Reference Material. Material that is stable within the measuring range of temperature is selected as a reference for comparison with a sample. The name of a selected material is described.

(5) Container. A sample and a reference material are put into an appropriate container for measurement. The material and the shape of the container are described.

(6) Pressure. The pressure of purde gas in the measurement device is described as either “normal” or “high”.

(7) Others. Items other than the ones listed above are described in the form of a pair of an item name and its value. An example could be the mass and thickness of a sample.

2.4. Measurement Result. The result of measurement is not needed directly for setting up measurements conditions. However, it is an essential component of thermal analysis and provides useful information by itself. It is described in list form as follows

(endothermic/exothermic, peak-shift, height,
measurementTemperature, range, peakArea,
thermalCharacteristics)

where “endothermic/exothermic” means that one of the two is specified, and “peak-shift” means that one or both of the two is specified, “height” is the maximal height of the peak, “measurement temperature” represents the range of temperature in which thermal characteristics are observed, and “range” represents the range of temperature where peak-shift is observed.

2.5. Bibliographical Items. The source information of a case such as a title, pages, the name of a journal or book, is described. Bibliographical information is included in a case as a component part because most cases are collected from journals, monographs, and handbooks.

Table 2 summarizes the representation scheme of a case as explained above. Cases are actually stored in the form of an attribute−value pair.

3. ONTOLOGY

3.1. Thesaurus. As detailed in the previous section, various terms are used to describe a case, such as a sample name, a class name, or an attribute name. The problem here is that any alternatives can refer to an identical object. A thesaurus, which defines synonyms, superordinate, subordinate, and related terms, is provided, since it allows TASC to use terms freely and retrieve cases using *is-a* relation or association among related terms. While the relationships among concepts defined in the thesaurus could be considered items in the concept dictionary detailed below, the thesaurus is installed as an independent dictionary by extracting the relationships between concepts, that is, inclusion, equivalence, and association. In addition, this thesaurus is equipped with the definitions of terms which represent qualitative values of attributes. For instance, the terms such as “little”, “small”, “large”, “much”, “thin”, “thick”, “low”, or “high” are used to express quantity or form; a certain order relation holds among those terms. Although they might not be strict in their classification, they permit a loose matching of attribute values.

3.2. Classification Tree. In TASC, polymeric materials are classified hierarchically from the viewpoint of chemical structures, forming a decision tree, which is called a classification tree in this system. Each internal node of the tree corresponds to the category of a material. A part of the classification tree is shown in Figure 2. For instance, the term “polyethylene” in Figure 2 corresponds to the node of class name “polyethylene”, whose parent node represents the superordinate concept “polyethylene group”. Leaf nodes of the classification tree represent the names of specific materials. The classification tree is used for the identification of similar cases during case retrieval and for user interface to select and specify appropriate class names.

3.3. Concept Dictionary. The information about polymeric materials commonly used in the field of thermal analysis is organized as a concept dictionary, which corresponds to so-called ontology.[7] The descriptive unit of the dictionary is the category which is an immediate superordinate concept of specific materials, corresponding to the parent of a leaf node in the classification tree. This manner of selecting the descriptive unit relies on the fact that the categorical concept provides more useful information needed for thermal analysis than the concept of specific materials. The following descriptors are given:

(1) Class Name. The lowest category of classification hierarchy, corresponding to the class name of sample information, such as “low-density polyethylene”.

Table 2. Attributes of a Case Representation and Their Forms of Values

attribute	form of values
measurement purpose	
A-purpose	sentence in English e.g., "The estimation of thermal expansion of... "
C-purpose	list of terms representing thermal characteristics: (term-l, term-2, ...)
sample information	
sample name	any name of a sample. e.g., PET
class name	category name into which the sample is classified e.g., LDPE
constitution	constitutive relation of the sample: relation (constituent-1, constituent-2, ...)
producing process	list of producing steps in terms of five descriptors: $((s_1, p_1, m_1, t_1, d_1)\ (s_2, p_2, m_2, t_2, d_2)\ ...)$
form	term representing the sample's form e.g., block, film, bar, yarn, ...
measurement conditions	
measuring device	DTA, DSC
temperature program	$((t_s, t_e, h_s, d_n)\ ...)$
purde gas	[name of the gas, rate of flow (mL/min)]
reference material	name of the material
container	(name of the material, shape)
pressure	normal, high, pressure (kg/cm^2)
[mass]	mass (mg)
[thickness]	thickness (mm)
measurement result	
endothermic/exothermic	"endothermic", "exothermic"
peak/shift	"peak", "shift"
height	maximal height of a peak
temperature	temperature range of any thermal characteristics: (t_2, t_2)
range	temperature range of a peak or a shift (t_1, t_2)
area	area of a peak
characteristics	(characteristic-1, characteristic-2, ...)
bibliographical items	author, title, journal/book, date, pages

(2) Phase. The phase that a material takes according to temperature changes is described as a list whose members are placed in ascending order of temperature, for example, (glass, gum, crystal, melting).

(3) State. The phase state at normal temperature, one of the states of the phases mentioned above, is described. For example, "crystal" is the state of "low-density polyethylene".

(4) Properties. Physicochemical properties or features are described as attributes of the category in the list form of attribute−value pairs. For example, the properties of low-density polyethylene are described as follows:

((crystallization, low) (shockproof, high) (waterproof, moderate)
(chemicalResistance, high) (electricProperty, good) (coldProof, fair))

(5) Use. The use of the materials belonging to the category is described in list form. Each use is expressed both in general terms such as "industrial film" and in concrete terms such as "bucket". For example, the use of "low-density polyethylene" is described as follows:

(thinFilm, industrialFilm, agriculturalFilm, cap, artificialFlower, sealedContainer, kitchenItem, bucket, pipe, tank, stationary, toy, fishingNet, rope, cloth, tape, keroseneCan, drumCan, electricPart)

(6) Chemical Structure. The structure of a repeating unit is described. Therefore, the class name as a descriptive unit of the concept dictionary is determined uniquely with respect to the repeating unit.

For example, the description for LDPE (low-density polyethylene) is given in the concept dictionary as follows:

className:	(LDPE, low-density polyethylene)
phase:	(glass, crystal, gum)
property:	(crystallizationDegree, low)
	(shockproof, high)
	(waterproof, good)
	(chemicalResistance, high)
use:	(film, commodity, paper, container, electricPart)
chemicalStructure:	$-(CH_2\ CH_2)-$

The cross-referring relations among the sample names and class names of the case base, the classification tree, and the concept dictionary, are shown in Figure 3. The leaf nodes of the classification tree correspond to the sample names of cases and so do the class names of the classification tree to those of cases and the concept dictionary.

4. SIMILARITY DEFINITION

In order to perform a similar-case retrieval, it is a central task to define the similarity between a problem and a case. The case of thermal analysis is represented from two points of view, sample information as a material and measurement purpose, as explained before. On the other hand, the information known about a new problem is of the sample itself and the measurement purpose. Thus, the similarity between a problem and a case should be defined with respect

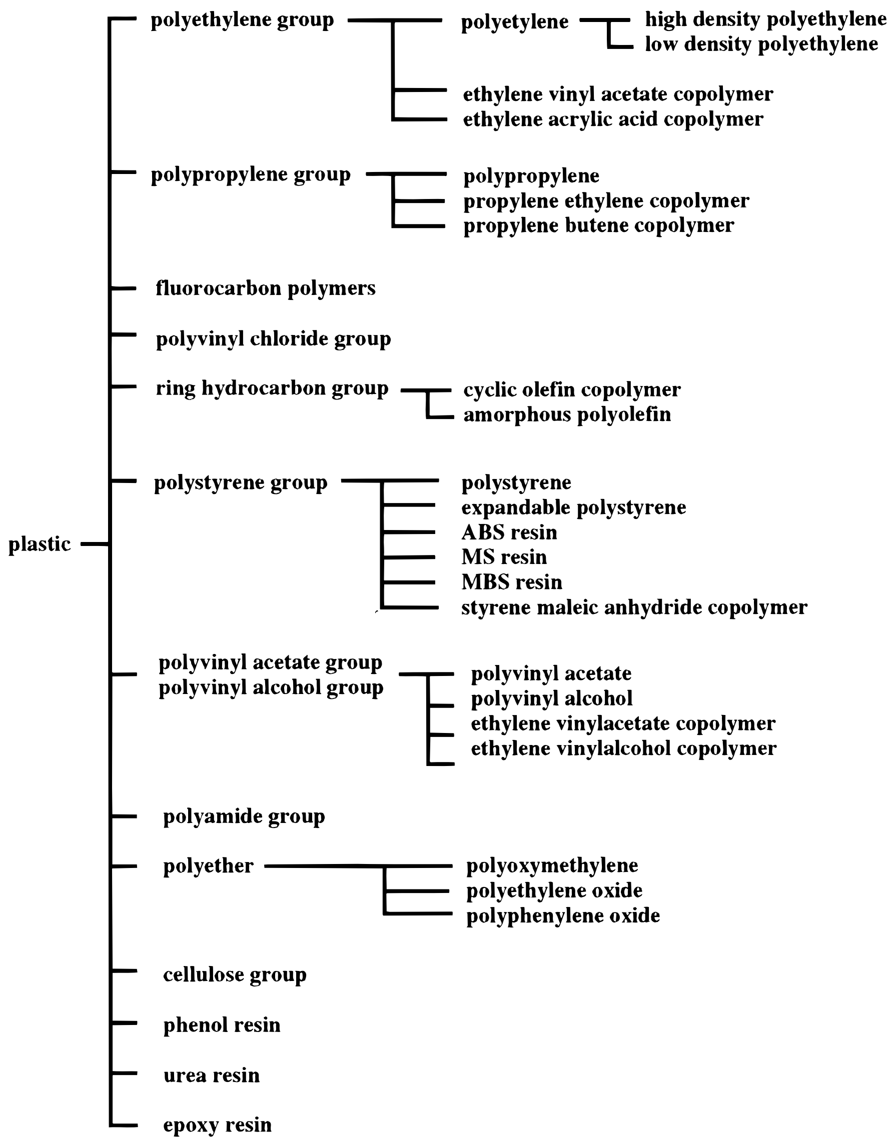

Figure 2. A part of the classification tree is shown, which gives the hierarchy of plastics. Each node of the tree represents the class name of a certain group of plastics.

to the two viewpoints: sample information and measurement purpose. Furthermore, the similarity is elaborated as follows.

The similarity of sample information is defined hierarchically in three levels of abstract: the level of sample names (denoted by S_1^S), the level of class names (denoted by S_2^S), and the level of properties (denoted by S_3^S). This means that the lower level definition expresses the concrete similarity of a material as a whole, whereas the higher-level definition expresses the abstract or partial similarity in the form of an attribute set. The hierarchical definition of similarity allows flexible case retrieval. Each of the similarities is computed as a score S_i^S, and the case matched at the lower level and with higher score is interpreted as a more similar case, which is defined below.

The similarity of measurement purpose is defined in two ways: the viewpoint of A-purpose (denoted by S_1^P) and the viewpoint of C-purpose (denoted by S_2^P). When the case retrieval is performed with respect to the measurement purpose, S_1^P is preferred to S_2^P.

Supposing that S is a set of cases obtained by retrieval of S_i^S and P is a set of cases by retrieval of S_i^P, then the final set of similar cases is given by $S \cap P$. The entire structure of the similarity definition is shown in Figure 4.

4.1. Similarity of Samples as Materials. A. Level of Sample Names. A case with the same sample name is viewed as a similar case. The similarity score is defined as follows:

$$S_1^S = f_0 + \sum_{i=1}^{3} w_i f_i$$

where f_0 is a base score, and the subscript i indicates that ith item of a sample information (i = 1, 2, 3, corresponding to constitution, production process, and form, respectively); f_0 is a base value for sample name matching; f_i represents the matching degree of ith item (i = 1, 2, 3); w_i is the weight of f_i, which is given according to the measurement purpose. For instance, if a measurement purpose is “glass transition”, the corresponding weights (w_1, w_2, w_3) = (1, 1, 0) may be given, which means that the form item (i = 3) does not affect measuring glass transition. These weight vectors are stored in TASC as one of the knowledge bases (actually, parameter

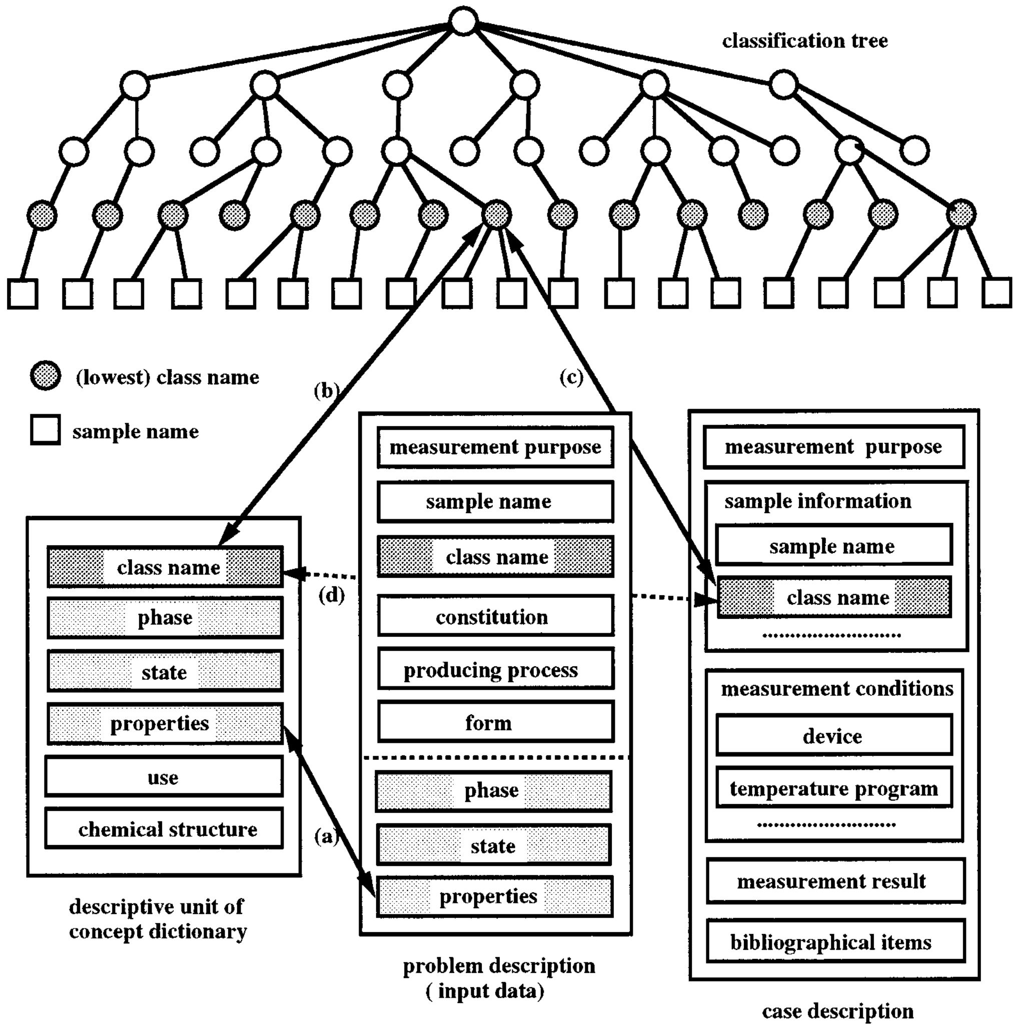

Figure 3. The cross-referring relations of class names among the classification tree, the concept dictionary, and the case base are shown. For example, if the class name of an input problem is not found in the case base, the property (including phase and state) of the problem is looked up in the concept dictionary. If found, the class name of the concept dictionary, or its superordinate class name in the classification tree, is used instead of the one specified in the problem, and it is searched for in the case base. This flow of retrieval is shown in the figure as a, b, c, and d.

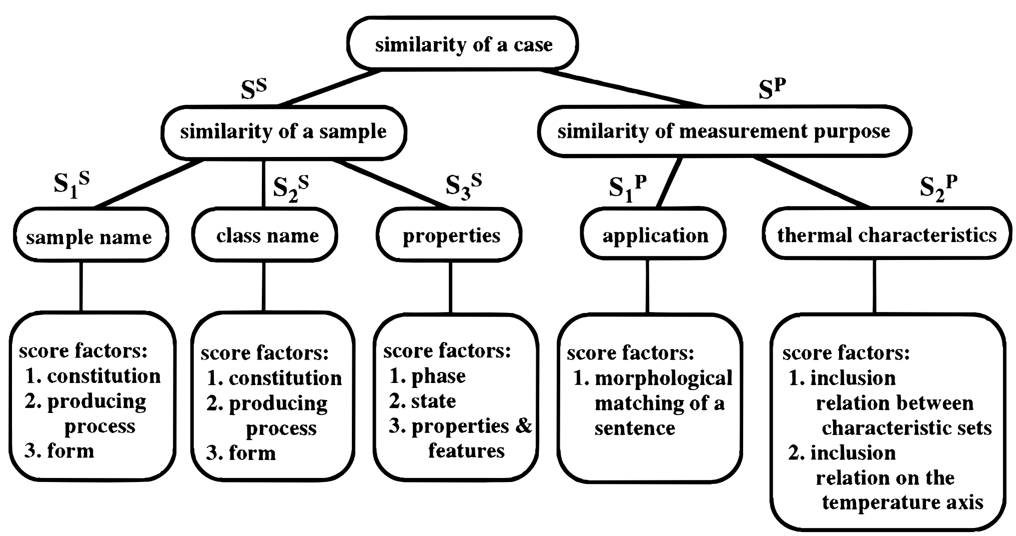

Figure 4. The hierarchical structure of the definition of similarity is shown. The similarity between a problem and a case is evaluated if the occasion arises during the case retrieval, so not all kinds of the similarity are computed for each problem.

lists). Thus, the definition of S_1^S includes information related to measurement purpose, and therefore, the similarity of sample information is not independent of that of measurement purpose. The value f_i is computed as follows, where synonyms and related terms in the thesaurus are employed through a matching process.

(a) Constitution (f_1). It is the degree of matching with respect to the constitution of samples. The descriptors of the constitution are constituents and the relation between them, as explained before, implies that the matching should be carried out for all of the descriptors. However, the value is computed only if the sample names are identical, which means that the constituents of the samples are also identical. Therefore, f_1 is defined as follows:

$$f_1 = \begin{cases} 1, & \text{if } C^P = C^C \\ 0, & \text{if either } C^P \text{ or } C^C \text{ has no description} \\ -1, & \text{otherwise} \end{cases}$$

where C^P and C^C indicates the constitutional relation of a problem and a case, respectively. If a sample consists of only one constituent, the constitutional relation can be viewed as "single", which is one of the cases $C^P = C^C$ (i.e., $f_1 = 1$). For example, if both the constitution of a problem and a case are given as follows

blend (polystyrene, poly-2-chlorostyrene)

then $f_1 = 1$, because $C^P = C^C = \textit{blend}$ and the constituents are the same.

(b) Production Process (f_2). The matching degree of each step of the production process of a problem and a case is computed. The steps in which a starting material and a product are the same for the problem and case are extracted. Then, the matching degree is computed using three parameters: processing method (m), temperature (t), and duration (d) for each step. Finally, f_2 is obtained as the sum of those matching degrees. Thus, f_2 is defined as follows, supposing that (s^P, p^P, m^P, t^P, d^P) and (s^C, p^C, m^C, t^C, d^C) represents a production step of a problem and a case, respectively:

$$f_2 = \sum(\delta(m^P,m^C) + r_t + r_d)$$

where Σ indicates the sum of matching degrees explained above, and $\delta(m^P,m^C)$, r_t, and r_d are computed as follows:

$$\delta(m^P,m^C) = \begin{cases} 1, & \text{if } m^P = m^C \\ 0, & \text{if } m^P \text{ or } m^C \text{ is not described} \\ -1, & \text{otherwise} \end{cases}$$

$$r_t = \begin{cases} 1, & \text{if } t^P \approx t^C \\ 0, & \text{otherwise} \end{cases}$$

$$r_d = \begin{cases} 1, & \text{if } d^P \approx d^C \\ 0, & \text{otherwise} \end{cases}$$

where each of $\delta(m^P,m^C)$, r_t, and r_d is set to zero if any of the values in the expression is undefined. Values r_t and r_d represent the matching degree of processing temperature and duration, where conditions $t^P \approx t^C$ and $d^P \approx d^C$ are defined empirically, and they are also set to zero unless $\delta(m^P,m^C)$ is 1.

(c) Form (f_3). The similarity of a sample's form is computed. The form is described by terms such as film and powder. Therefore, the similarity is defined as follow:

$$f_3 = \delta(\text{form}^P,\text{form}^C) = \begin{cases} 1, & \text{if form}^P = \text{form}^C \\ 0, & \text{otherwise} \end{cases}$$

where $\textit{form}^P$ and $\textit{form}^C$ represent the terms used for describing forms of samples.

B. Level of Class Names. When case retrieval fails to find cases with the same sample name, searching for cases with the same class name is tried alternatively. That is, the case with the same class name is viewed as a similar case. Full matching of class names or *is-a* reasoning using the thesaurus is performed in searching for class names. The score S_2^S is defined as follows:

$$S_2^S = f_0 + \sum_{i=1}^{3} w_i f_i$$

This definition is the same as that of sample name level. So are the terms w_i and f_i.

C. Level of Attributes. When case retrieval fails to find cases with the same class name, searching for cases with similar attribute values is tried. However, attribute values of samples are not described in the case base. Therefore, the attribute values of the problem are matched with those of the concept dictionary, and a class name is inferred as a matched concept, which is in turn searched for in the case base. As mentioned before, the class name of the concept dictionary is also the parent of a leaf node of the classification tree. Therefore, superordinate class names could be used for case retrieval instead of the class names found in the concept dictionary. The similarity score of attribute level is defined as follows:

$$S_s^S = \sum_{i=1}^{3} w_i g_i$$

where $i = 1, 2, 3$ indicates items of a descriptive unit of the concept dictionary: phase, state, and property, respectively. g_i represents the matching degree of the ith item, i.e., the score. w_i is a weight given according to measurement purpose. The value of w_i is either 1 or 0; value 1 is assigned to w_i, if g_i is affected by the measurement purpose; value 0 is assigned otherwise. The weight vector (w_1, w_2, w_3) is also stored in the knowledge base of TASC.

The score g_i is computed as follows, using the thesaurus as the computation of f_i.

(1) Phase (g_1). The score g_1 is given by the following expression:

$$g_1 = \text{the number of matched elements}$$

The phase is represented in the form of a list whose elements are terms such as glass, gum, or crystal. The score is the number of matched terms between the problem and a category of the concept dictionary, for example, $g_1 = 3$ for lists (glass, gum, crystal, melting) and (glass, crystal, melting).

(2) State (g_2). The score g_2 is computed as follows, when $g_1 > 0$.

$$g_2 = \begin{cases} 1, & \text{if the states at normal temperature are the same} \\ 0, & \text{otherwise} \end{cases}$$

For example, two states "glass" and "crystal" give $g_2 = 0$; two states "glass" and "glass" give $g_2 = 1$.

(3) Property (g_3). The score g_3 gives the similarity of properties and features of the problem and a category (i.e., descriptive unit) of the concept dictionary, defined as follows:

$$g_3 = \text{the number of attributes of the same value}$$

For example, the score $g_3 = 4$ for LDPE (low-density polyethylene) and HDPE (high-density polyethylene), which is the number of attributes of the same value (i.e., shockproof, waterproof, chemical-proof, and electric characteristics, as seen in Table 3.)

4.2. Similarity of Measurement Purpose. A. Application Purpose. The application purpose (A-purpose) of measurement is expressed by a sentence in English, so whether two A-purposes are similar or not is determined by the semantic similarity of the corresponding two sentences. However, a simple definition of the similarity is employed here, since it is difficult to discriminate the meaning of sentences. That is, two A-purposes are the same only if the corresponding two sentences morphologically match:

$$S_1^{\mathrm{P}} = \begin{cases} s^{\mathrm{A}}, & \text{if two sentences match exactly} \\ \text{unknown}, & \text{otherwise} \end{cases}$$

where s^{A} is a similarity score given experimentally. If $S_1^{\mathrm{P}} = s^{\mathrm{A}}$, it is used as the similarity of measurement purpose, without evaluating the similarity of C-purpose. If $S_1^{\mathrm{P}} =$ unknown, the similarity of C-purpose is computed, described below.

B. Purpose in Terms of Thermal Characteristics. Two kinds of definitions are provided for C-purpose: (1) definition based on the inclusiveness between sets of thermal characteristics, and (2) definition based on the inclusiveness between temperature range. Supposing that T^{P} and T^{C} indicate sets of thermal characteristics respectively representing C-purposes of a problem and a case, T^{P} is interpreted basically as similar to T^{C}, if $T^{\mathrm{P}} \subseteq T^{\mathrm{C}}$. On the other hand, if thermal characteristics are mapped to a temperature axis, an order relation between the corresponding peak positions always holds. Thus, the inclusiveness in terms of the order relation can be defined on the temperature axis. For instance, since crystalline polymers have the state of a crystal, the thermal characteristic appears in the order of glass transition, crystallization, and melting on the temperature axis. This situation is shown in Figure 5a. If the order relation holds for all the crystalline polymers, T^{P} is interpreted to be similar to T^{C} in spite of $T^{\mathrm{P}} \cap T^{\mathrm{C}} = \varnothing$, where

$$T^{\mathrm{P}} = (\text{crystallization})$$

$$T^{\mathrm{C}} = (\text{glassTransition, melting})$$

This is because the temperature range for measuring T^{C} is considered to include the range needed for measuring T^{P}. This relation between T^{P} and T^{C} is expressed as follows:

$$T^{\mathrm{P}} < T^{\mathrm{C}}$$

Table 3. Properties and Features of LDPE (Low-Density Polyethylene) and HDPE (High-Density Polyethylene)

property/feature	LDPE	HDPE
crystallinity	low	high
shockproof	good	good
waterproof	fair	good
chemical-proof	good	good
electric property	good	good
coldproof	fair	
rigidity		fair
surface strength		high
softening temperature		low
acid-resistant		fair
alkali-resistant		fair
solvent		soluble

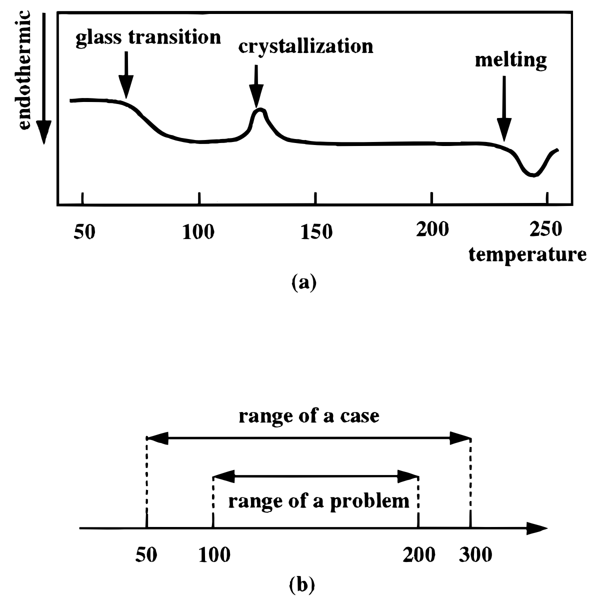

Figure 5. Panel a is an example of a thermal analysis chart of polyethyleneterephthalate, where three thermal characteristics are ordered on the temperature axis. Panel b shows the inclusion relation of temperature ranges for the measurement of the crystallization temperature of a problem to that of the glass transition and melting temperatures of the above case.

Figure 5b shows this situation. Therefore, a problem is interpreted to be similar to a case if either $T^{\mathrm{P}} \subseteq T^{\mathrm{C}}$ or $< T^{\mathrm{C}}$ holds. That is, the similarity score S_2^{P} of T^{P} for T^{C} is defined as follows:

$$S_2^{\mathrm{P}} = \begin{cases} s_1^{\mathrm{C}}, & \text{if } T^{\mathrm{P}} = T^{\mathrm{C}} \\ s_2^{\mathrm{C}}, & \text{if } T^{\mathrm{P}} \subset T^{\mathrm{C}} \\ s_3^{\mathrm{C}}, & \text{if } T^{\mathrm{P}} < T^{\mathrm{C}} \\ 0, & \text{otherwise} \end{cases}$$

where s_1^{C}, s_3^{C}, and s_3^{C} are similarity scores given experimentally.

5. METHODS

The whole system constitution is shown in Figure 6. The case retriever, difference recognizer, and case modifier perform similar case retrieval, difference recognition between a problem and a case, and case adaptation to the problem, respectively. The case retriever consults the classification tree, thesaurus, and concept dictionary when retrieving the case base; the difference recognizer and case modifier consult

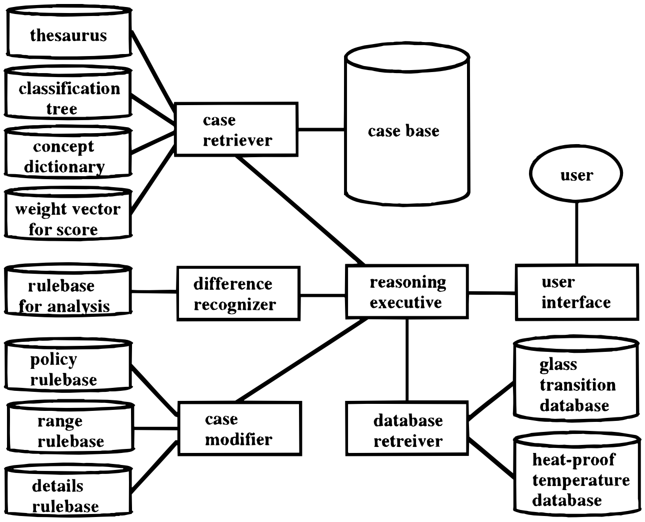

Figure 6. The system configuration of TASC is presented. The reasoning executive module located at the center of the figure controls the whole system. The case analyzer is not located explicitly in the figure, but is replaced with the difference recognizer and reasoning executive.

rule bases and databases accordingly. The overall process of TASC is as follows:

(1) Input a problem in the form of sample information and measurement purpose. Input items are a sample name, a class name, constitution, production process, form, A-purpose, and C-purpose.

(2) Retrieve similar cases. The similarity is evaluated with respect to the sample information and measurement purpose as explained above. The classification tree, concept dictionary, and thesaurus are used if necessary for matching or reasoning. A prototype measurement condition is generated from the retrieved cases.

(3) Recognize and extract the differences between the problem and the cases. Additional information may be required to input.

(4) Modify the prototype to adapt the problem according to the differences extracted. Knowledge bases and data bases are consulted for the adaptation.

(5) Output the measurement conditions obtained as a result, which should be tested by actual measurement.

Some of the procedures unique to TASC are detailed below.

5.1. Similar Case Retrieval. The procedure of similar case retrieval is as follows.

(1) Search by Sample Names. If a sample name is specified in the problem given, the cases of the same name are searched for in the case base. All the cases found in this manner make a set of candidate cases, S^{A}. Then, step 2 is followed.

(2) Search by Class Names. A class name is always specified in the problem, and the cases of the same class name are searched for in the case base regardless of the result of previous search by sample names. All the cases retrieved like this make a set of candidate cases, S^{B}. Making a set $S = S^{A} \cup S^{B}$, if S is not empty, step 4 is followed; otherwise, step 3 is followed.

(3) Search by Properties in the Concept Dictionary. If properties and features are specified in the problem, the categories (i.e., descriptive units of the concept dictionary) matched with them are searched for in the concept dictionary. If several categories are found, the category with maximal similarity S_3^{S} is selected among them, and its class name is employed as a retrieval target. Then, it is necessary to go back to step 2. This process is repeated if the search by the class name in step 2 fails, until all the class names are tried. When no categories were found, the case retrieval fails.

(4) Search by A-Purpose. If a sentence expressing the application purpose of the measurement is specified in the problem, morphological matching of the sentences is performed for the cases in the set S. The case whose A-purpose matches exactly is selected as a member of a candidate set R. If no cases matched with the problem, step 5 is followed.

(5) Search by C-Purpose. The similarity of the problem to the case in the set S is evaluated with respect to C-purpose. That is, whether $T^{T} \subseteq T^{C}$ or $T^{P} < T^{C}$ holds is checked. If so, the case is selected as a member of the candidate set R. After all the cases in S are checked, step 6 is followed.

(6) Selection of Probable Cases. The members of the candidate set R are the cases that are similar to the problem from both viewpoints. The next process follows according to the size of set R. (a) If $|R| = 0$, the case retrieval fails. (b) If $|R| = 1$, one member of R is selected as a similar case. (c) If $|R| > 1$, the similarity S_1^{S} or S_2^{S} is computed for the members of R. The case with the maximal similarity is selected as a similar case, where S_1^{S} and S_2^{S} are not discriminated because they give the same kind of similarity.

(7) Derivation of a Prototype of Measurement Condition. A prototype of measurement condition for the problem is derived from the one or more selected probable cases.

5.2. Difference Recognition. The difference between a problem and a derived prototype is recognized with respect to both sample information and measurement purpose. Since a class name is supposed to be the same, the difference of sample information is checked on four items: sample names, constitution, production process, and form. The difference of measurement purpose corresponds to the types of similarity between the two sets of thermal characteristics T^{P} and T^{C} mentioned in the previous section. That is, there is no difference if A-purpose matches or $T^{P} = T^{C}$ holds for C-purpose. The difference is extracted when $T^{P} \subset T^{C}$ or $T^{P} < T^{C}$ holds for C-purpose.

5.3 Modification. The retrieved similar case is modified so that it adapts to the problem according to the sample information and measurement purpose. The modification proceeds by invoking production rules whose condition-parts match with the extracted differences. The rules are classified into three levels on the basis of the degree of generalization: (1) basic policy, (2) range of values, and (3) details. Table 4 shows the classification, where blank fields indicate the absence of rules. The hierarchical structure of the rule base brings about flexible setting of measurement conditions. For instance, even if the reasoning at detail-level fails and the measurement condition cannot be determined specifically, the results of the reasoning at higher level, that is, at the levels of basic policy or range of values, are available as useful advice for users.

A. Basic Policy Rules. The rule of this level gives a basic policy for setting up measurement conditions specified as its action, provided that sample information and measurement

Table 4. Classification of Contents of Modification Based on Rule Hierarchy[a]

measurement condition		basic policy	value range	details
measuring device		DTA, DSC		
temperature program	step	set up, not set up		
	start temperature	lower than standard, higher than standard	offset value, numeric range	numeric value
	end temperature	lower than standard, higher than standard	offset value, numeric range	numeric value
	heating rate	decrease slowly, increase slowly, etc.	numeric range	numeric value
	retention time	necessary, unnecessary	numeric range	numeric value
reference material		necessary, unnecessary	stable in the measuring range	
container	material	stable to the sample		material's name
	shape		open, closed	
purde gas	kind of gas		oxidative, corrosive, reductive	
	flow	static, dynamic	numeric range	numeric value
pressure		normal, high, low	numeric range	numeric value
other	mass	more, less	numeric range	numeric value
	thickness	thick, thin	numeric range	numeric value
	diameter		numeric range	numeric value
	form		block, film, bar	

[a] The symbol '|' indicates the selection of one of the contents.

purpose are specified in its condition-part. Some examples are shown below.

Policy for starting temperature:

if ((className, polymerBlend) and

(C-purpose, glassTransition) and

(phaseState, onePhase))

then ((get (glassTransitionTemperature, const-1, const-2))

(set (glassTransitionTemperature, lowerThan, middle (gtm-l, gtm-2))))

Policy for heating rate:

if ((className, plastic) and

(C-purpose, glassTransition))

then (increase (heatingRate))

where const-1 and const-2 mean two constituents, and gtm-1 and gtm-2 their glass transition temperature.

B. Rules for Deciding the Range of Values. The ranges of numerical values of measurement conditions are given as an intermediate form of specialization in these rules. If a range cannot be expressed by numerical values, the appropriate terms may be used instead, giving a qualitative expression. In the following example, the action-part of the range rule "increase heating rate" is specialized as one of the condition-parts of the basic policy rule shown above.

Rule for deciding the range of heating rate:

if ((className, plastic) and

(increase (heatingRate))

then (range (heatingRate, 10, 20))

C. Rules for Deciding Details. Measurement conditions are determined numerically as precisely as possible by these rules. While the items of the measurement conditions are listed in Table 2, they are not always independent of each other. Therefore, a value has to be decided consistently with the values already determined. If a measurement condition is included in the condition-part of a rule, the consistency is assured automatically because the rule requires that its condition-part matches the measurement condition already determined. In the following example, the range of a mass of a sample is specified in the condition-part of the rule, and the value thus satisfies the consistency restriction if the mass of the problem and the one specified here are the same, that is, a mass less than 5 mg.

Rule for deciding the details of heating rate:

if ((className, plastic) and

(mass, lessThan, 5))

then (set (heatingRate, 20))

6. RESULTS

6.1. Similar Case Retrieval. The case base consisting of 46 cases shown in Table 5 is prepared for the experiment of TASC. A-purposes are described to discriminate the cases in Table 5. The base score f_0 of S_1^S and S_2^S are 3 and 2; and the weights w_l, w_2, w_3 for both S_1^S and S_2^S are 2, 1, and 1, respectively. The similarity scores of A-purpose and C-purpose are given as $s^A = 3$, $s_1^C = 3$, $s_2^C = 2$, $s_3^C = 2$. The result of similar case retrieval for each member of the case base on the basis of leave-one-out method is shown in Table 6, where the field of C-purpose is divided into three according to the matching pattern between thermal characteristic sets: $=$, $\subset$, and $<$. That is, symbols "$=$", "$\subset$", and "$<$" indicate the exact matching between thermal characteristic sets, the inclusion relation between thermal characteristic sets, and the inclusion relation between temperature ranges, respectively. Six fields in Table 6, that is, sample names, class names, A-purpose, and three C-purposes, give ID numbers of similar cases retrieved with respect to the corresponding item. For example, when case 16 is picked up as a problem, three cases (ID numbers 17, 18, and 45) are retrieved, where all of them have the same sample name, and cases 17 and 18 are matched with respect to A-purpose, and case 45 with respect to C-purpose ($<$) from the view point of measurement purpose. Their similarity scores are indicated in the rightmost field as 6, 6, and 3, respectively,

Table 5. Forty-Six Measurement Cases in the Case Base[a]

ID	grp	cases (A-purpose)	ID	grp	cases (A-purpose)
1	1	absorptive water of cellulose	24	7	glass transition of polystyrene
2	1	absorptive water of rayon fiber	25	8	thermal history of nylon fiber
3		water in hollow fiber	26	8	thermal history of nylon fiber
4		water in polymeric absorbent	27	8	thermal history of nylon fiber
5		crystallization of lignin	28	8	thermal history of nylon fiber
6		crystallization of biodecomposable polyurethane	29	8	thermal history of nylon fiber
7		substitution degree of cellulose derivative	30		hardening reaction of hardening and prepolymer
8	2	print suitability of gum	31		enthalpy relaxation of PET
9	2	print suitability of gum	32	9	thermal properties of PBT
10	3	blend degree of union	33	9	thermal properties of PBT
11	3	blend degree of union	34		liquid phase separation of polymer blend
12	3	blend degree of union	35		glass transition of polymer alloy
13		oxygen barrier of EVOH copolymer	36		crystallization of polymer blend
14	4	thickness distribution of polyethylene crystal	37		heat resistance of aromatic polyamide
15	4	thickness distribution of polyethylene crystal	38		thermal properties of PEEK
16	5	heat stability of polyethylene	39		glass transition of aromatic polyether
17	5	heat stability of polyethylene	40		melting of liquid crystal polymer
18	5	heat stability of polyethylene	41		thermal properties of BR/SBR polymer blend
19	6	melting curve of isotactic polypropylene	42		thermal properties of conducting polymer
20	6	melting curve of isotactic polypropylene	43		melting process of nylon 66
21	6	melting curve of isotactic polypropylene	44		glass transition of gum
22	7	glass transition of polystyrene	45		thermal properties of polyethylene polypropylene polymer blend
23	7	glass transition of polystyrene	46		thermal properties of PET

[a] There are nine groups of measurements for the same purposes, such as ID number lists (1, 2), (8, 9), (10, 11, 12), and so on, indicated by the same group (grp) numbers.

in the order of ID numbers. It is shown that case 4 is found as a similar case when case 3 is given as a problem, whereas the inverse is not shown. That coincides with the fact that the matching pattern of case 3 search is C-purpose (<). The number of retrieved similar cases for cases 25, ..., 29, and 43 is relatively large because they are members of a measurement group for "nylon". Likewise, the number of retrieved similar cases for cases 34, 35, and 41 is large, because their class names are "polymer blend" which is commonly found in the case base.

The same experiment was carried out for the new problems shown in Table 7, where AP, CP, SN, CN, CF, PP, and FM indicate A-purpose, C-purpose, sample name, class name, configuration, preparation process, and form, respectively. The experiment was carried out in two ways: (a) a case with the same sample name is included in the case base (46 cases) and (b) a case with the same sample name is excluded from the case base (45 cases). The results are shown in sections a and b of Table 8. For the results of experiment a, the cases listed in the sample name field are the ones with the same sample name, and they have the largest similarity score indicated by boldface, which is the result expected. The sample names of the problems and cases with the largest similarity score are shown in pairs in Table 8c, which gives major difference between problems and retrieved cases.

6.2. Modification Based on Recognized Differences. The prototype measurement conditions and the results of adaptation for the similar case retrieved for experiment b mentioned above are shown in Table 9, which are proposed to users. The prototype is formed from the similar case retrieved and default conditions for plastics. Default conditions in prototypes are not modified through adaptation process. The following are knowledge and rules applied to the modification of the prototypes. Heading numbers of these rules correspond to the ones written in the rightmost field of Table 9:

(1) if (className is different)
  then (prefer default value of the problem's className)

Actually, this task is performed by looking up the table whose entry has fields of a pair (className, C-purpose) and temperature range, which is common knowledge to thermal analysis.

(2) if (className is "polymer blend")
  then (if (p1.c is near to p2.c)
    then (decrease heatingRate half))

where p1.c and p2.c are peak positions of a thermal characteristic (glass transition in this case) of component-1 and component-2 in a polymer blend. P1, p2, and c are instantiated when the rule is evoked.

(3) if (sample is highly hygroscopic)
  then (set purdeGas "nitrogen flow")

This is provided as empirical knowledge.

As a result, an appropriate measurement condition is obtained for each problem which oftentimes misled beginners to erroneous condition values. Of course, the successful adaptation depends entirely upon the quantity and quality of the knowledge base, and the experiment shown here is a successful example.

7. CONCLUSION

The CBR-based system, TASC, which assists general users in setting up the measurement conditions of thermal analysis has been developed and tested for the case base of 46 cases and three problems. As a result, it has been shown that intended cases are exactly retrieved on the basis of the similarity defined in this paper and that the correct measure-

Table 6. Results of Similar Case Retrieval Based on the Leave-One-Out Method in the 46 Cases

				C-purpose			
ID	sample name	class name	A-purpose	$=$	$\subset$	$<$	similarity
1		2		2			5
2		1		1			5
3		4			4		2
8		9		9			5
9		8		8			5
10		11,12	11,12				5,5
11		10,12	10,12				5,5
12		10,11	10,11				5,5
14		15	15				5
15		14	14				5
16	17,18,45		17,18			45	6,6,3
17	16,18,45		16,18			45	6,6,3
18	16,17,45		16,17			45	6,6,3
19		20,21	20,21				5,5
20		19,21	19,21				5,5
21		19,20	19,20				5,5
22		23,24	23,24				5,5
23		22,24	22,24				5,5
24		22,23	22,23				5,5
25	26	27,28,29,43	26,27,28,29	43			5,6,5,5,3
26	25	27,28,29,43	25,27,28,29	43			5,5,5,5,3
27	28,29,43	25,26	25,26,28,29	43			6,5,6,6,4
28	27,29,43	25,26	25,26,27,29	43			5,5,6,6,4
29	27,28,43	25,26	25,26,27,28	43			5,5,6,6,4
31		32,33			32,33		4,4
32		33,38		33,	38		5,5
33		32,38		32	38		5,5
34		35,36,41,45		35,41	36,45		2,1,2,1
35		34,36,41,45		34,41	36,45		2,1,2,1
36		45		45			3
37		39		39			5
38		32,33		32,33			5,5
39		37		37			5
40		32,33,38				32,33,38	4,4,4
41		34,35,36,44,45		34,35,44	36,45		2,2,2,4,2
43	27,28,29	25,26		25,26,27,28,29			3,3,4,4,4
44		41		41			4
45		36		36			3
46		32,33			32,33		4,4

Table 7. Three Problems Used for Testing Similar Case Retrieval and Adaptation

problem ID	problems
1	AP: thermal properties of PS/P2ClS polymer blend CP: glass transition SN: PS/P2ClS blend polymer, polystyrene/ poly-2-chlorostyrene blend polymer CN: polymer blend, polymer alloy CF: PP: FM:
2	AP: thermal properties of PBT CP: melting SN: PBT, polybutylene terephthalate CN: engineering plastic CF: PP: FM:
3	AP: thermal history of nylon 6 CP: melting SN: nylon 6 CN: nylon, thermoplastic polymer CF: PP: FM:

ment conditions have been proposed by generating and modifying prototypes from retrieved similar cases. In TASC, a measurement case of thermal analysis is represented from the two viewpoints of sample information as a material and measurement purpose. The similarity of thermal analysis cases is defined on the basis of the two viewpoints accordingly. The ontology consisting of a thesaurus, a classification tree, and a concept dictionary is provided to allow flexible usage of various names and expressions in the case representation and reasoning process. Being located at the middle of memory-based reasoning and rule-based reasoning, as mentioned in the introduction, CBR can be viewed as a kind of analogical reasoning[9] that treats specific information as well as general rules. It seems suitable to employ CBR as a reasoning framework for the problem of setting up measurement conditions of thermal analysis because of the following reasons. Firstly, there is much lack of data in measurement cases, although desired items are prepared to represent measurement cases of thermal analysis. Secondly, the style and description level of the actual reports and articles of thermal analysis measurements are not regulated, and they are described in various expressions and ranges. Thirdly, an algorithmic method for setting up measurement conditions of thermal analysis is not known so far. Therefore, if a simple RBR is, for example, employed as a reasoning mechanism, condition-parts of rules do not match with most actual problems, which the former implementation of this system demonstrates.[16] The similar situation occurs oftentimes in

Table 8. Results of Similar Case Retrieval for the Problems 1−3

(a) Results When the Case with the Same Sample Name with the Problem is Included in the Case Base

ID	sample name	class name	A-purpose	C-purpose			similarity
				=	⊂	<	
1	**34**	35,36,41,45		**34**,35,41	36,45		**7**,2,2,3,2
2	**32**,33	38	**32**,33		38		**6**,5,4
3	**25**,26	27,28,29,43,46		**25**,26,27,28,29,43,46	4		**5**,4,4,3,3,4,5

(b) Results When the Case with the Same Sample Name with the Problem is Excluded from the Case Base

ID	sample name	class name	A-purpose	C-purpose			similarity
				=	⊂	<	
1		35,36,**41**,45		35,**41**	36,45		2,2,**3**,2
2		**38**			**38**		**4**
3		27,28,29,43,**46**		27,28,29,43,**46**			4,3,3,4,**5**

(c) Sample Names of the Problems and the Cases with the Largest Similarity, Which Makes the Major Differences Between the Problems and the Similar Cases

problems' sample names	cases' sample names
PS/P2ClS polymer blend	BR/SBR polymer blend
PBT	PEEK
nylon 6	PET

Table 9. Prototypes of Measurement Conditions Generated by the Similar Cases Retrieved and Default Measurement Conditions for Plastics and the Modified Ones from Them[a]

problem/case	items	prototype	result	rule
P1/C41	start temperature	−120	**rt**	**1**
	end temperature	rt	**150**	**1**
	heating rate	10	**5**	**2**
	purde gas	⟨air, static⟩	air, static	
	container	Al pan	Al pan	
	mass	⟨10⟩	10	
P2/C38	start temperature	rt	rt	
	end temperature	400	**300**	**1**
	heating rate	10	10	
	purde gas	⟨air, static⟩	air, static	
	container	Al pan	Al pan	
	mass	⟨10⟩	10	
P3/C46	start temperature	rt	rt	
	end temperature	280	280	
	heating rate	10	10	
	purde gas	air, static	**nitrogen, flow**	**3**
	container	Al pan	Al pan	
	mass	⟨10⟩	10	

[a] For example, a notation P1/C41 represents that the prototype for P1 (problem 1) is set up from C41 (case 41), and so on. Values enclosed by brackets are the ones filled with defaults. Modified values are indicated by boldface.

various problems, so combinations of RBR and CBR are proposed as a kind of aproach.[8,10,11] TASC employs CBR and introduces the classification tree, thesaurus, and concept dictionary to achieve flexible matching. That is, in case retrieval, candidate cases are collected roughly by matching sample names, class names, and measurement purposes at the terminology level, where the terms are identified in the ontology. Then, the candidates are ordered according to the similarity scores. Similar cases selected in this manner are modified using various knowledge and data. That implementation of ontology and knowledge bases seems to give flexibility and robustness of matching and reasoning.

TASC has been tested about similar case retrieval with respect to 46 measurement cases and has retrieved similar cases exactly as expected. Three problems have been tested to see if their measurement conditions are correctly reasoned, and the results are satisfactory ones. These results suggest that the representation and similarity definition of measurement cases are adequate and that the underlying ontology and knowledge bases works effectively. TASC is a prototype system which implements only a small case base, ontology, and rule bases, and the similarity definition is rather loose. However, the results obtained by the experiments suggest that the CBR approach is prospective. That is, TASC has a possibility to evolve into a practical system with a large-scale case base, an appropriately organized ontology, and knowledge bases.

REFERENCES AND NOTES

(1) Kanbe, H.; Ozawa, T. *Thermal Analysis* (in Japanese). Kodansha: Tokyo, **1992**.

(2) The Japanese Thermal Analysis Society *Handbook of Calorimetry and Thermal Analysis* (in Japanese); Maruzen Publishers: Tokyo, 1998.

(3) Research Group for Applied Thermal Measurement of The Japanese Thermal Analysis Society *Applied Thermal Analysis* (in Japanese). Nikkan Kogyo Shinbunsha: Tokyo, **1996**.

(4) Kolodner, J. Case-Based Reasoning; *Morgan Kaufmann Publishers*: San Mateo CA, 1993.

(5) Aamodt, A.; Plaza, E. *Case-Based Reasoning: Foundational Issues, Methodological Variations, and System Approaches, AICOM* **1994**, *7*, 39−59.

(6) Ashley, K.; Simoudis, E. Case-Based Reasoning: Issues and Applications (Tutorial). *13th National Conference on Artificial Intelligence,* 1996.

(7) Leake, D. B. *Case-Based Reasoning*; AAAI Press: Menlo Park, CA, 1996.

(8) Kobayashi, S. Present and Future of Case-Based Reasoning. *J. Jpn. Soc. Artificial Intelligence* **1992**, *7*, 550−566.

(9) Matsubara, H. Case-Based Reasoning as a Mechanism for Reasoning and Learning, *J. Jpn. Soc. Artificial Intelligence* **1992**, *7*, 567−575.

(10) Branting, L. K.; Porter, B. W. Rules and Precedents as Complementary Warrants. *Proceedings Ninth National Conference on Artificial Intelligence*, 1991, pp 3−9.

(11) Golding, A. R.; Rosenbloom, P. S. Improving Rule-Based System through Case-Based Reasoning. *Proceedings Ninth National Conference on Artificial Intelligence*, 1991, pp 22−27.

(12) Hatakeyama, T.; Quinn, F. X. *Thermal Analysis: Fundamentals and Applications to Polymer Science*; John Wiley & Sons: Chichester, 1994.

(13) Mahot, V. B. F. (Ed) *Calorimetry and Thermal Analysis of Polymers*; Hanser Publishers: Munich, 1994.

(14) Tanaka, K.; Nishimoto, Y.; Nakayama, T. Computer-Assisted Thermal Analysis System Based on Case-Based Reasoning. *Proceedings of the 19th Symposium on Chemical Information*, 1996, pp 41−44.
(15) Research Group for Polymer Analysis of The Japanese Analytical Chemistry Society *Handbook for Polymer Analysis*; Kinokuniya Shoten Publishers: Tokyo, 1995.
(16) Tanaka, K.; Nishimoto, Y.; Murakami, K. Computer-Assisted Compound Analysis −2. *Tokyo Symposium on Devices and Systems for Analytical Chemistry*, 1995, pp 65−66.

CI980160I