unrelated project provided the chemical information is made easily accessible.

VI. CONCLUSIONS

In this paper, we have described how Sgroups can be used to dramatically extend representation of chemical structures in computer programs. In the Substance Module, chemical Sgroups are used to represent, store, and search polymers, biopolymers, mixtures, and formulations. A more general class of data Sgroups was also implemented which permits the user to add properties to the connection table and have them searchable as an integral part of the structure.

ACKNOWLEDGMENT

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Improvements in Derwent Plasdoc System†

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The Plasdoc Code has undergone many changes, culminating in the introduction of Key Serial Numbers in 1978. Further development along the same path is not possible, so with subscriber agreement Derwent began a major revision. Plasdoc subscribers were involved from the start in the design. Initially a questionnaire was sent out to ascertain the problem areas; later an Advisory Group was formed consisting of nine Plasdoc users and representation by the Japanese Plasdoc Association. The main requirements were continuity with the old code, extendability, no significant change in coverage, retention of the hierarchical nature, and linking between related terms to make searching more specific. The enhanced code comprises greatly extended nonstructural codes; Specific Compound Numbers for chemicals, which for polymer formers are embedded in a hierarchy of generic terms based on the current system; Chemical Aspects terms for generic structure searches; and levels of linking via proximity operators.

BACKGROUND

It was 25 years ago that Derwent introduced the Plasdoc Code in order to handle polymer information in the patent literature. In the beginning the Plasdoc Punch Code, as it was known in those days, was based on a punch card containing 80 columns and 12 rows which represented a maximum of 960 possible punch positions for encoding data. Due to this limit to the number of such positions available, groups of punch positions were used to represent concepts, and this multiple usage led to poor relevance in searching.

Take, for example, the concept "acetate", which is represented by the single punch position 067. In order to create a code for the concept vinyl acetate, 067 was combined with the punch position vinyl carboxylic esters (066); for the concept cellulose acetate, 067 was combined with three other punch positions cellulosics (252), modified polymer (231), and esterification (239).

In 1976 the punch-card system was loaded on-line with each punch position being represented by an alphanumeric code, derived from its coordinates on the card. Several modifications and improvements took place over the years, including in 1977 the addition of codes for all the elements, but this was achieved by the combination of punch positions to create the extra codes required. Such a system is unavoidably prone to false drops if separate indexing ideas are expressed on the same "card records", since spurious combinations of codes can be recovered.

1978 saw the most dramatic of these modifications with the creation of Key Serial numbers (KS). These were assigned to precoordinated groups of punch codes. Thus, a key serial was created for propylene homopolymer, ethylene binary copolymer, phenol monomer, and so on. Key serial numbers were also assigned to some concepts such as "carbon black light stabiliser" and "glass fibre filler". The obvious benefit of these key serials was the ability to search specifically for those combinations of concepts to which they had been applied. However, since key serials were unique to each concept, they

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did not fit into a hierarchical structure, and generic searching was still only possible using the punch codes, which from 1978 onward were autogenerated from the key serial numbers.

In 1982, the introduction of a few bound terms for the commonly occurring copolymers and condensation polymers took place, and in 1984, Plasdoc Registry Compounds with corresponding Registry Numbers were incorporated. These Registry compounds consisted of approximately 750 compounds commonly occurring as additives and catalysts in polymers and for the first time enabled these compounds to be retrieved specifically in Plasdoc.

PRELIMINARY STUDIES

Work began in earnest on enhancing the Plasdoc Code in 1987. We began by consulting the users. Initially, a questionnaire was sent out to all Plasdoc subscribers to ascertain the major problem areas, inviting suggestions on ways to improve these areas, and also to ask for ideas on how to develop the new system as a whole. The questionnaire was followed by visits to several of the companies to investigate their comments in further detail.

The general response was interesting and enlightening but too diverse to provide a foundation to build upon directly. Few of the capabilities needed could be achieved in the short term, and it was decided that a major enhancement of the system was the only practical solution.

In spite of the ambiguous and diverse results of the questionnaire, it was clear that suggestions, ideas, and comments from the people who actually use the Plasdoc Code were vital to build a system which would meet the needs of technology today and in the future. At the 1988 subscribers' meetings, satellite sessions were held on the Plasdoc problem. At these meetings, the concept of an Advisory Group was proposed. By the autumn of 1988, the Plasdoc Advisory Group had been formed. The Group consists of 10 participants; 5 from the U.S., 4 from Europe, and a representative from the Japanese Plasdoc Association. Together the members of this group, each a specialist in his or her own field, represent a broad spectrum of polymer chemistry and plastics technology.

Three meetings were held, the last of which took place late in 1989, and these produced the basic framework for developing the Plasdoc enhancements.

Main Aims of the Enhancements. As a result of all this consultation, the following priorities for the enhancement were decided:

1. Increase the number of specific polymer formers—in the current system there are fewer than 200 specific monomers and condensants.
2. Improve the ability to handle low molecular weight compounds.
3. Expand the nonstructural terms.
4. Provide linking between related terms. This will increase the specificity for copolymer searching, by linking polymer formers within a polymer.
5. One item specified by the majority of users was to provide continuity with the existing code. This will include retaining the same coverage as at present and also retaining the hierarchical structure of the code.
6. Design a system which is easy to expand in the future. An especially interesting future option is the use of graphical indexing to improve the handling of certain chemical features.

From the beginning of the study on the Plasdoc enhancements, the majority of users were in favour of continuity between the existing system and the new system. Since the key serials are prelinked and nonhierarchical, it was impossible to start with them as our basis. However, by retracing our steps back to the original punch-position definitions, it was found that they would provide the basic framework for us to build upon. Wherever possible, these original concepts, within their hierarchies, are present in the enhanced code, so that it will be possible to convert the old coding to the new.

MAIN FEATURES OF THE ENHANCEMENTS

1. Expansion of the range and variety of specific chemicals searchable, by the use of Specific Compound Numbers for all common specific polymer formers and low molecular weight compounds.
2. A system of generic chemical terms called Chemical Aspects to handle generic structure information.
3. Hierarchical structure, incorporating as far as possible the existing hierarchies, with autoposting of broader terms when narrow terms are indexed.
4. Multi-tier linking to associate related terms together.
5. Comprehensive Thesaurus containing all searchable terms and synonyms, indicating relationships between terms and scope notes to aid in searching.

The system has been divided into two areas: the first for chemical structure handling of all chemical information and the second for nonstructure handling or nonchemical information. These in turn are divided into a number of areas of interest or "Facets".

CHEMICAL STRUCTURE HANDLING

Specific Compound Numbers. We identified a large number of individual chemicals which are not specifically retrievable in the present system but which are commonplace and of commerical interest. These chemicals were suggested by a variety of sources, including customer requests, proposals generated by the coding staff, and statistical studies of compound occurrences. Each individual compound has been assigned a Specific Compound Number (SCN). A system of reusable compound identifiers for common compounds, Specific Compound Numbers, is already implemented in Derwent Sections BCE for Markush DARC indexing, and by adopting this system for use in Plasdoc we are moving toward a unified coding method for chemicals. In cases where SCN's do not already exist for compounds which occur in Plasdoc, these will be created and added to the Specific Compound Number series.

Chemical Aspects. In addition to the generic codes and Specific Compound Numbers, a system of Chemical Aspects has been created. This is one of the major improvements provided by the enhancements. The Chemical Aspects, somewhat similar to those used by the American Petroleum Institute, consist of:

Generic terms—inorganic, organic, hydrocarbon, ...
Generic subunits—aliphatic, unsaturated aliphatic chain, single ring alicyclic, bicyclic heterocyclic, ...
Number of rings present—1, 2, 3, 4, ≥5
Atoms in heterocyclic ring—N, O, P, >1 S, >1 N, ...
C-C unsaturation—no unsaturation, acetylenic, diolefinic, terminal olefinic, ...
Broad functionality types—salt, ester, acid halide, metal-C, ...
Carbon count—1C, 2C, 3C, ... 12C, >12C
Specific functionality terms—epoxide, mercaptan, amine, diamine, azide, ether, phenolic, sulphonyl, isocyanate, ...
Elements and their periodic groups

The Chemical Aspects have been introduced in order to provide more chemical information for those compounds which cannot be covered by a Specific Compound Number. The indexing of generic concepts and Markush structures will both benefit from the use of these aspects. In the present system,

there are only a few chemical multifacet terms which serve this function. A detailed system of autoposting has also been devised whereby each Specific Compound Number will autopost the relevant Chemical Aspects. This will enable very generic searching to be carried out based on aspects alone.

Structural Section. The structural section contains all the chemical information. The following facets make up the structural section.

Polymer Formers: The polymer formers facet contains concepts for monomers and condensants such as ethylene, methyl methacrylate, propylene oxide, and phosgene.

Low Molecular Weight Compounds: The low molecular weight compounds facet contains all those compounds which commonly occur as additives and catalysts in polymers and plastics. This includes compounds such as carbon black, benzoyl peroxide, titanium trichloride, and 2-hydroxy-4-methoxybenzophenone.

Natural Polymers: The natural polymers facet contains such compounds as starch, alginic acid, various cellulose ethers and esters, and several rather poorly defined compounds such as bituminous materials.

Polymer Types: Polymer types are generic descriptions of polymers, basically without regard for the materials or methods of preparation. Examples are polyesters, polyamides, polyimides, and polyurethanes. Structure definition here is at the level of the repeating unit.

In order to retain the hierarchical structure for polymer formers, it has been necessary to create two facets—polymer formers and low molecular weight compounds—but fully defined compounds within these two facets will be handled using the same methods, whether they are polymer formers, additives, or catalysts. The distinction between polymer formers and low molecular weight chemicals that are not polymer formers is somewhat artificial and is only required for continuity with the existing code and the retention of the generic concepts for broad types of monomer and condensant which form an important part of that code. It is also proposed to extend the existing coverage to include the indexing of modifying agents for polymers and to use SCN's to represent these compounds.

Handling Polymers. Different methods of handling the different types of information available have had to be adopted. A polymer can be defined in terms of its starting materials, the product, or both. The starting material(s) can be defined in terms of individual compound(s), generic descriptors of a class of compound, Markush structure, or combinations of these. Likewise the formed polymer can have a fully defined structure or only a partially or generically defined structure, which is sufficient to enable it to be assigned to a class of polymer.

Where the information is available, the policy of indexing polymers in terms of the polymer formers—monomers and condensants—will continue. For the situations where the polymer formers are not known, we will use the term Structural Repeating Unit (SRU) along with polymer types and chemical aspects as applicable.

As mentioned previously, retention of the hierarchical structure of the system was high on the list of priorities. This is especially important in the polymer formers facet for generic searching. For that reason, we took the existing hierarchical framework and, apart from minor modifications and rationalisation, expanded it by incorporation of several hundred more specific terms for polymer formers.

Within each hierarchy, we have a main generic, such as monoolefinic, containing other hierarchies for example vinyl aromatics monoolefinic. This hierarchy contains individual polymer formers, for example, α-Methyl styrene and Cinnamic acid. In addition, there is a need for "semigeneric" concepts for certain classes of polymer formers such as Halomethyl styrenes. These in turn may also contain specific concepts, in this case Chloromethyl styrene and Bromomethyl styrene. Within any hierarchical system, it is necessary to cater for individual concepts which have not been incorporated. Thus, "Other vinyl aromatic monoolefinic" will be used for new specific compounds or those compounds which occur infrequently and do not fit elsewhere within the vinyl aromatics monoolefinic hierarchy.

SCN and new generic codes	Concept	Exactly corresponding punch codes
G0022	Monoolefinic	—
	:	
G0099	Vinyl aromatic monoolefinic	055
R00708	Styrene	055 056
R90003	Vinyl toluenes	055 057
	:	
R00673	α-Methyl styrene	055 058
G0102	Halomethyl styrenes	—
R90004	Chloromethyl styrene	—
R90005	Bromomethyl styrene	—
R01416	Cinnamic acid	—
	:	
G0146	Other vinyl aromatic monoolefinic	—

Figure 1. Extract from hierarchy with codes.

Each generic concept and semigeneric concept has been assigned a "generic code" and each specific concept in the polymer formers hierarchy has been assigned a Specific Compound Number (SCN) as applied in WPI-Markush DARC (WPIM). Any given term within a hierarchy will autopost the corresponding broader term(s) within the hierarchy. All the specific compound numbers will also autogenerate the chemical aspects. For the generic concepts some chemical aspects will be autogenerated, but more can be applied during indexing if the information is available. Figure 1 shows an extract from the hierarchies with proposed codes, either SCN or generic codes, for the concepts. Where these concepts are exactly equivalent to concepts in the existing system, the punch codes have been indicated.

Thus, in the above example, α-Methyl styrene, Halomethyl styrenes, Cinnamic acid, and Other vinyl aromatic monoolefinic will all autopost the code for vinyl aromatics monoolefinic, which in turn will autopost monoolefinic.

The versatility of this system allows for a compound such as α-methylstyrene to be searched specifically by its SCN, generically via the vinyl aromatics monoolefinic hierarchy, or generically using chemical aspects; the Chemical Aspects in this case for α-methylstyrene are organic, hydrocarbon, unsaturated aliphatic chain, benzene ring, monoolefinic, terminal olefin, and 9C.

Each of the specific concept within a hierarchy will autopost the appropriate wider generic term(s). These autoposted terms will be distinguishable from the terms which have actually been indexed. This will provide the option of searching for instances where the generic has been specifically indexed, to retrieve those patents which describe a concept only at the generic level. Comprehensive retrieval for a given concept can, therefore, be achieved by searching for the "indexed" generic concept in addition to the specific concept, without the risk of retrieving records where the generic term has been autoposted by a different specific concept. A search for the generic can retrieve references which have been specifically indexed together with those which have been autoposted.

Handling Low Molecular Weight Compounds. The existing coverage of low molecular weight compounds is restricted to a few generic terms, a few specific chemicals, and the Plasdoc registry compounds. We have enlarged the list of individual compounds which can be retrieved specifically, and these will

now be searchable linked to their functions, e.g., calcium carbonate filler.

These additives and catalysts will be handled in the same way as polymer formers by using SCN's. The current Plasdoc registry has been enlarged, and SCN's will be used in place of the Registry numbers. As with polymer formers, it is intended that the low molecular weight compounds will autopost their chemical aspects.

Within the Low Molecular Weight Compounds facet, there are small local hierarchies, for example, there is a generic "iron oxide" term and several narrower terms for individual iron oxides. However, there is not such a complete set of hierarchies as there is for the polymer formers, since no such system exists already, and because it would not be workable in the more diverse field of additives and catalysts.

NONSTRUCTURE HANDLING

Nonstructural Section. The nonstructural section contains all the nonchemical information. The following facets make up the nonstructural section:

Novelty descriptors
Multifacet
Composition
Shape and form
Additive functions
Catalyst functions
Chemical processes
Physical operations
Equipment
Properties
Applications

Most of the nonstructural facets are equivalent to sections in the current system. However, in certain ones of these, the content or coverage has changed.

In the new system, the Multifacet section now contains only nonchemical information, and these concepts will be searchable with concepts from any other facet. Thus, "in-situ", a concept within this facet could be searched with foaming process, polymerization process, or production of an additive within a polymer.

The Composition facet contains the equivalent of the old punch-code terms for homopolymer, monomer, etc. with additional new concepts, for example, grafting monomer.

The Shape and Form facet now caters for shape and form of additives and catalysts as well as polymers.

Additive and Catalyst facets now contain only functional concepts for additives and catalysts—the chemical information will be found in the low molecular weight compounds facet and can be searched by linking the function and the compound.

The nonstructural terms have been expanded, in many cases by the splitting up of combined or precoordinated concepts to provide access to the simpler, more basic terms. In the cases where, for example, a positive and a negative property shared the same code, these have now been divided to create two separate concepts with different codes. The Key Serial 2628 represents at least six concepts, including flexibility, stiffness, and Young's modulus. Each of these concepts now has an individual code.

As stated previously we have retained the hierarchical structure and expanded it where necessary, and as in the chemical section, broader terms are automatically generated when narrow terms are indexed.

LINKING

The introduction of the many new concepts will obviously improve specificity, but we also intend to introduce a method of linking in order to improve the efficiency of searching. It is very important to be able to indicate associations between concepts in indexing and to search with these associations. For example, it should be possible to connect the chemical identity of an additive with its activity, e.g., a phenolic compound as an antioxidant. For a polymer, the monomers forming the polymer should be connected. For the combination of an additive with a polymer, some way is needed to indicate that a particular additive goes with a certain polymer and not other polymers mentioned in the patent, which are, e.g., other layers in a laminate. This was the reason why the Key Serials were devised—they consist simply of ready-made combinations of the more fundamental concepts contained in the old punch code. The potential permutations are of course vast, and this is one reason why we did not want simply to create more key serial numbers. The problems are made worse by the fact that patents commonly indicate a variety of alternative substances for a given function, as either a Markush, a list of substances, or a series of examples. Therefore, we decided not to create more ready-made combinations of concepts, like the KS, but to use linking flexibly to indicate the associations between simple terms.

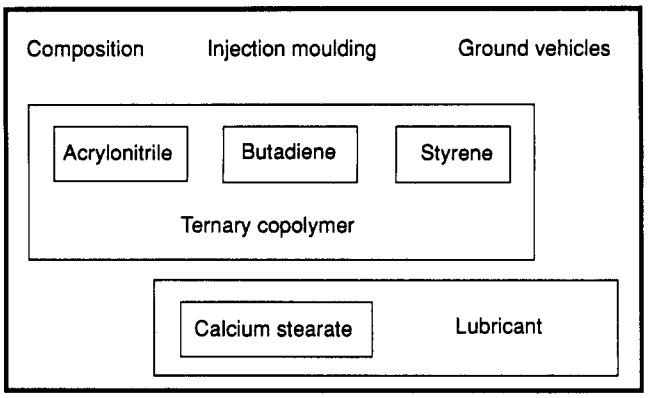

Figure 2. Depiction of linking levels: ABS with calcium stearate for injection molding of automobile parts.

Three basic classes or levels of linking are envisaged.

1. Linking aspects to generic terms (+SCN) to define a substance.
2. Linking a substance with activity or use—as additive, catalyst component, or monomer.
3. Linking a (class of) substance with a (class of) substance.

These three levels of linking in the order given widen in scope—each is wider than its predecessor. There is a parallel with the way language text is arranged in an "ideal" paper—each sentence announces a fact; several sentences combine to form a paragraph describing a particular facet of the subject; and the collection of paragraphs defines the subject of the paper.

Pursuing the parallel, it seems feasible then to have each substance defined by a "sentence" of indexing; to associate alternative substances with their activity in "paragraphs", so we have a paragraph about each functional class of substance; and out of these paragraphs to build "chapters" about related classes of substances.

Essentially, we have described an extended form of the "proximity" operations that all the on-line hosts now offer, and we believe these can form the basis for the three tiers of linking which are intended.

This is a rather subtle concept, best illustrated by an example (see Figure 2). This example of ABS containing a calcium stearate lubricant injection molded to form automobile parts represents a simplified view of the linking levels and the concepts to be linked. The smallest boxes, which are equivalent to the first level of linking, each contain a compound and all the information used to represent that compound (SCN or

R90087 **Cotton** [*natural polymer*]
BT Cellulose
BT Cellulosics

R01186 **Coumarone** [*polymer former*]
BT Non-vinyl aromatics monoolefinic
BT Monoolefinic
UF Benzofuran

{Coupling agent} [*additive*]
USE Adhesion improver D033

N4853 **Cracking** [*property*]
NT Environmental stress cracking
NT Stress cracking
BT Stress-strain properties
BT Mechanical properties
UF Crazing
UF Fracture surfaces

N8899 **Crates** [*application*]
BT Containers
BT Packaging

{Crazing} [*property*]
USE Cracking N4853

Figure 3. Thesaurus sample.

generic code and aspects). These smallest boxes can be linked at the second level to their function. In the example the monomers are linked to each other and to the concept ternary copolymer at this level. Also calcium stearate is linked to lubricant at this level; if there were other lubricants they too would be linked to "lubricant" in the same way. At the third level (the largest box), these classes of chemicals are linked together and linked to the concepts for injection molding, ground vehicles, and composition.

THESAURUS

To aid searching, a Thesaurus will be produced containing all main terms and synonyms in alphabetical order and will be fully cross-referenced.

The relationships between concepts within a hierarchy are indicated by the labels BROADER TERM (BT) and NARROWER TERM (NT). Synonyms are indicated by USED FOR (UF) and USE terms. Some terms are followed by SEE ALSO (SA) references to suggest other areas of related or similar technology. Scope notes have been incorporated where appropriate to indicate the extent or limitations of the concept. All of these features will be displayed within the Thesaurus (see Figure 3). In addition to the Thesaurus, there will be a hierarchical listing of all the concepts. This will display the relationships between concepts within a facet.

ACKNOWLEDGMENT

We thank all members of the Plasdoc Advisory Group for their assistance and support in the design of the new system and look forward to working with them during the β-testing. We also thank Joe Aggarwal and all members of the Derwent Plasdoc Coding Department, who have been continually involved in the enhancements, making suggestions, compiling statistics, and testing. At present, they are involved in in-house testing of all elements of the new system.

The IFI Polymer Indexing System: Its Past, Present, and Future†

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IFI/Plenum, producer of the CLAIMS online U.S. patents files, uses a unique system for indexing polymers based on their identification in terms of logical starting materials, broad classes defining the repeating units, and very often, descriptive concepts and polymer names. In addition, the Comprehensive Database (CDB), available by subscription, makes use of a special set of roles applied to the monomers to indicate that the material being indexed is polymeric in nature. These codes are linked to the monomers to indicate their claimed function and whether postmodification, such as crosslinking, has occurred. The system thus allows for polymer retrieval at both specific and generic levels. Examples of this indexing system are illustrated and some possible future linking enhancements for improving the precision and selectivity of polymer retrieval are discussed.

INTRODUCTION

Just the mention of the word "polymer" has been known to strike fear into the hearts of mere mortals and certainly, at the least, a sense of apprehension, if not foreboding, to an information searcher. The word itself sounds innocuous enough. After all, a polymer appears to be nothing more than a compound of very high molecular weight. What can be so menacing about such highly regarded materials as polyethylene or nylon or even, for that matter, the much maligned polystyrene? A searcher undoubtedly has nothing against polymers personally, except when it is time to search the literature for a specific one. Then these polymers seem to develop almost human-like "attitude problems". They either become very timid, not wishing to be found at all (i.e., no retrieval) or they run in large "gangs" and hope for anonymity in the crowd (i.e., many false drops). The key to finding the best way of tracking down these sometimes elusive quarries is to know their habitat (the system used to index them) and become familiar with their upbringing (the historical continuity of that index system).

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