

our two services, but I am confident that with good will on both sides some means of preventing duplication will be worked out between us in the not too distant future for the mutual benefit of all concerned.

In order to give widest possible access to its patents files, Derwent is going to the expense of putting them up on three different online hosts, two of them in the U.S. It is regrettable that neither U.S. host will be allowed also to mount the INPADOC, EPO, or JAPATIC patents files—nor will they be

allowed to mount the CAS abstracts. Unless these barriers can be overcome, the dream of being able to interrogate the world's major patents databases at one and the same time on a single host computer will not be possible.

My hope is that, if ever I am privileged to talk to the Chemical Information Division of the ACS again, I shall be able to report that this dream has come true—and that you in this Division have played an important part in its achievement.

## Polymer Patent Information Systems Could Be Even Better!<sup>†</sup>

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Patents that involve polymers are a very substantial portion of the patent literature. Both Derwent Publications and IFI/Plenum have highly developed systems for indexing polymer patents, and significant features relating to polymers (though not restricted to patents) are found in other databases, most notably *Chemical Abstracts* and the CAS Registry. This paper surveys some strengths and limitations of today's systems and looks toward possible future advances.

### INTRODUCTION

Patents that involve polymers constitute a very substantial portion of the patent literature. *Plasdoc*, the section devoted to polymers, is by far the largest component of the chemically related patents in Derwent's *Central Patents Index* or CPI. Since 1981, nearly one-third of the patents in the CPI have been assigned to *Plasdoc*, averaging nearly 850 basic patents (first-abstracted members of patent families) per week during 1984.

Polymers have a huge economic importance. In the U.S., sales of plastics alone exceeded 18 million metric tons in 1983; the figure does not include elastomers and other types of polymer. It is essential to provide this enterprise with timely and accurate documentation of polymer patents, for both current awareness and retrospective information retrieval.

Two information services are especially important for current awareness on polymer patents: the aforementioned *Plasdoc* and *Chemical Abstracts*. For retrospective retrieval these two are again of prime importance, along with the CLAIMS family from IFI/Plenum. Other files also contain polymer information but lack a specialized polymer retrieval system or are too limited in scope to be of general interest.

What must a polymer patent information service deal with? Figure 1 shows something of the scope that is needed. The range is enormous, involving not only chemistry and chemical engineering but also mechanical engineering, electrical engineering, physics, and other disciplines. And the complexity of the technology can be prodigious. A satisfactory information system must be able to describe the significant points of individual patents so that they can be retrieved reliably, with as much specificity as possible. With 40 000 or so new inventions involving polymers being added annually to what is already a massive heap, discrimination is essential to effective information retrieval.

Until about the mid-1960s there were no specialized information systems for polymer patents. *Chemical Abstracts* covered many of them, with an emphasis on the chemistry, and IFI's *Uniterm Index* indexed U.S. polymer patents. Then a lot of things began to happen. Chemical Abstracts Service

(CAS) developed its Registry system for chemical substances and applied it to many polymer systems. CAS also set out to encompass more of the technology of polymers through two special publications: *POST-J* for journal literature, *POST-P* for patents. Meanwhile, Derwent, which had recently started documentation services on pharmaceutical and agricultural chemical patents, began *Plasdoc* in 1966. Finally, du Pont started a highly sophisticated in-house patent indexing system in 1964, which was later modified and merged with IFI's *Uniterm* system to form the basis of IFI's *Comprehensive Data Base*, or *CLAIMS-CDB* as it is known in the online form.

### CURRENT AWARENESS SERVICES

Before considering the characteristics of the retrieval systems, let us look at the current awareness situation, with respect to timeliness and also abstract content. This is also an appropriate place to consider differences in coverage.

Derwent has always aimed at providing information as rapidly as possible. Derwent alerting abstracts for the most important patent-issuing bodies are normally in the hands of subscribers slightly less than 2 months after the publication dates of the patents. *Chemical Abstracts* was considerably slower, but has improved its timeliness to where it will cover these major countries about 1-2 months later than Derwent. A significant difference between the two, however, is that Derwent covers all of any country's output for a given week in a single week. There is no time distribution for any country in Derwent coverage. CA, on the other hand, does have a time distribution, so that, while the bulk of coverage in major countries is taken care of within about 4 months, there is inevitably a tail to the distribution that brings in some abstracts considerably later. Thus, one never knows when CA might have finished covering the patents issued on a given date.

For the Soviet Union the timeliness picture is reversed. Here, CA takes its abstracts from brief descriptions published by the Soviets (*Otkrytiya*, *Izobreteniya*), while Derwent waits to obtain full copies of Soviet patents to work from. As a result, CA's Soviet coverage runs some months ahead of Derwent's. Note, too, that CA enters listings for equivalent patents in its printed index very rapidly, more rapidly than Derwent, because of the input that it gets from INPADOC, the International Patent Documentation Center. CA does not

<sup>†</sup> Presented at the Herman Skolnik Award Symposium, Division of Chemical Information, American Chemical Society, Philadelphia, PA, Aug 28, 1984.

- Polymerization catalyst systems; initiators; modifiers
- Polymerization processes
- Polymer structure, composition
- Compounding agents, techniques
- Polymer modification reactions, processes
- Fabrication techniques, equipment
- Polymer shapes, forms
- Molecular and physical properties
- End uses
- Monomer preparation, purification

Figure 1. Scope of polymer patent information.

have listings of equivalents online, however, whereas Derwent does.

What about the contents of the respective abstracts? In most instances, I think that there is little comparison. I consider Derwent's documentation abstracts to be the most thorough and informative ones available.

Derwent produces two types of abstract: alerting and documentation. The alerting abstract tries to summarize the broadest and the more specific claims of a patent. It describes the patent's purpose and may add other points of interest. The documentation abstract goes beyond this to highlight what is new about the invention, to indicate where significant the full scope of the disclosure even beyond the claims, and usually to provide detailed examples with data and drawings when appropriate. Both abstracts are provided with a highly informative Derwent-written title.

Many Derwent abstracts from Japan have been significantly below the standard set for other countries; I often have to check CA for more detail on Japanese patents. However, Derwent has done a great deal during the past year or so to raise this standard. There are also times when a Derwent abstract gets tied up in the "legalese" of the language of a patent's claims. On the whole, though, Derwent's documentation abstracts are often good enough to serve as a surrogate for the full document.

CAS, on the other hand, has emphasized that its aim is not to provide a document surrogate but rather to lead one to documents that might be of interest. CA abstracts are usually well written and lucid but rarely provide the amount of information available from Derwent. Figure 2 gives an example of the typical differences between Derwent and CA abstracts. CA chose to describe a vapor phase run without indicating that all of the other runs were made in liquid hydrocarbon slurry. Little inkling is given of the possible range of the catalyst components, nor is there any indication that the catalyst was also used for the homopolymerization of ethylene. All of these points are shown in some degree by Derwent, but the example given by Derwent is incorrectly shown to be homopolymerization. It was in fact copolymerization with 1-butene, which should be obvious to a knowledgeable reader from the density of the product. Figure 3 provides another comparison, emphasizing the wealth of detail provided by Derwent. The generally high quality and thoroughness of Derwent's documentation abstracts are such that patent reports produced in our group typically consist in substantial part of Derwent documentation abstracts surrounded by commentary and analysis of the technology involved.

#### SUBJECT COVERAGE

*Plasdoc* also excels in the breadth of its subject coverage. My initial exposure to *Plasdoc* took place in 1967, when I became concerned that *POST-P* was covering only about 225 patents every two weeks,<sup>1</sup> while *Plasdoc* was averaging about

Table I. Patents Not Covered by CA

patent no.	subject matter
BE 894 191	heating system for platens of particleboard press
CA 1 136 498	adhering reflective beads to road signs
DD 156 673	glass fiber- and filler-containing polymer laminates
DD 156 681	silicone-coated ink transfer cylinder
DD 156 758	loudspeaker membrane coated with plasticized PVAc
DE 3 116 379	platen press for fiberboard manufacture
DE 3 119 563	polyethylene-coated compressible tube for paste medicines
DE 3 119 774	core polyester or polyamide yarn surrounded by split viscose fibers
DE 3 119 949	mixer for two-component adhesives and resins
DE 3 119 959	acoustically damped rail wheel using plastics strips
DE 3 120 014	injection molded knob
DE 3 121 225	cloth-mounted plastic foam insulation
DE 3 121 809	heating strip for plastics forming
DE 3 122 271	blister packaging machine
DE 3 122 462	elastic groin bandage for athletes
DE 3 122 601	rubber processing rollers
DE 3 122 792	winter tire with fiber bundles projecting from tread
DE 3 203 202	deep drawn box lid with gripping rim
DE 3 211 123	resin-coated dental prosthesis
DE 3 219 514	extruding wire-reinforced tubing
DE 3 219 640	plastics bushing in loom sley mounting for noise reduction
DE 3 220 046	silicone pushbutton with integral marking
DE 3 220 493	electrophotographic copier fixing roll with resin beads for surface roughness

400 each week. The gross differential that existed then has narrowed substantially, as CA has broadened its selection criteria, but CA still does not select numerous items that are covered by Derwent. The reverse is rarely true.

The differences in coverage are illustrated by checking the first 50 patents in a single *Plasdoc* issue, the first for 1983. Of those 50, 23 were not covered by CA, and are shown in Table I. They fall into essentially three categories: equipment for polymer processing, methods of polymer processing, and end uses. I am not implying that CA should have included most of these items. My point is rather to illustrate that there are substantial differences in coverage between *Plasdoc* and CA. Users should be well aware of those differences.

#### RETRIEVAL CAPABILITIES: CA

Let us look now at the retrieval capabilities of the various databases for polymer patents. Figure 4 shows the subject-access points available in the CA online files. An important point to keep in mind is that one should use not only Registry Numbers but also the names for substances, since sometimes only the name appears in the indexing record. For some polymers—notably synthetic rubbers—index entries are normally in the form of words rather than Registry Numbers. A valuable feature of some online versions of the CA file is the ability to use linking logic to ensure that the selected terms occur in the same context, thus avoiding retrieval noise. An example is given in Figure 5.

All of the access points can add effectively to a search strategy. Conspicuously missing to this date are the words in CA's abstract.

Certain aspects of CAS indexing policy are important to keep in mind and can create problems in searching CA. Until recently, CAS would index only examples backed by hard data and not index the patent's claims. Over the 1979–1982 period CAS has phased in the indexing of things claimed specifically, even if they were not fully exemplified. This policy falls short of needs in patents, which frequently feature broad generic claims that are not backed by data but can be very important for legal purposes. I have seen examples where a polymerization catalyst support critical to an invention was not indexed, apparently because it was not in itself the source of the catalytic activity. I have seen examples where a specific reactant

## A. Plasdac Alerting

ICIL \* A17 55436 D/31 \*EP -32-309  
 Olefin polymerisation catalyst component prepn. - by treating inert particles with organo magnesium cpd., halide and transition metal cpd.  
 IMPERIAL CHEM INDS LTD 11.12.80-GB-039757 (10.01.80-GB-000882)  
 (22.07.81) C08F-04/62 C08F-10  
 22.12.80 as 304678 (+ 6.6.80-GB-018582) (966RH) (E) No-Citns. E(AT BE CH DE FR GB IT LI NL SE)  
 Prodn. of a component (A) of an olefin polymerisation catalyst treating (a) inert, solid particles having reactive sites with (b) organo Mg cpd. or complex or mixt. of the organo Mg cpd. and an Al cpd., (c) H halide, B halide, halogen, interhalogen cpd. or halides of Gp IVB, VB or VIB elements and (d) transition metal (m) cpd. of formula M(Oa)(Rb)(X)n (where M is a Gp IVA, VA or VIA transition metal; X is halogen other than F; R is opt. subst. hydrocarbyl or gp. OR; R' is opt. subst. hydrocarbyl; b is 0 or number up to valency of M with the exception that when M is Ti, n is not 4; a is 0 or 1; b is 0 or number up to valency of M and 2a + b + n equals valency of M. A Lewis Base (V) may also be used in forming the catalyst component.  
 The olefin polymerisation catalyst is also claimed comprising component (A) and an organo-metallic cpd. of Gp IIA metal or of Al or a complex of an organometallic cpd. of Gp IA or IIA metal with an organo Al cpd.  
 The catalyst is esp. used to polymerise ethylene opt. mixed with a different olefin such as butene-1 in the gas phase. (45pp)

## B. Chemical Abstracts

95:151464s Olefin polymerization catalyst component. Caunt, Anthony David; Gavens, Paul David; McMeeking, John (Imperial Chemical Industries Ltd.) Eur. Pat. Appl. 32,309 (Cl. C08F10/00), 22 Jul 1981, Brit. Appl. 80/882, 10 Jan 1980; 45 pp. A catalyst component for the polymn. of olefins was prepd. by treating an inert solid particulate material with an org. Mg compd., a halogen-contg. compd., and a transition metal compd. Thus, 108 g SiO<sub>2</sub> was suspended in 800 cm<sup>3</sup> isoparaffin fraction, treated with 351 cm<sup>3</sup> 0.625 M MgBu<sub>2</sub> [1191-47-5] in isoparaffin fraction, stirred 4 h at 20°, decanted, washed 5 times, resuspended, treated with 500 cm<sup>3</sup> SiCl<sub>4</sub>, stirred 60 h, stirred 4 h at 80°, sepd., washed, treated with 21.8 cm<sup>3</sup> BzOEt [93-89-0] in 1 L isoparaffin fraction, stirred 2 h at room temp., decanted, washed suspended in 1630 cm<sup>3</sup> TiCl<sub>2</sub>iso-Pr<sub>2</sub> [762-99-2] at 80°, stirred 4 h, decanted, resuspended, filtered, and dried under vacuum at 50° to give a catalyst component. A 58.3:23.4:18.3 M mixt. of ethylene, 1-butene, and H was circulated continuously through a 20-cm-diam. fluidized bed reactor at 80° with Ti-catalyst component at 2.35 mmol/h and triisobutylaluminum [1070-00-4] at 12.5 mmol/h to give 1.45 kg/h copolymer [25087-34-7] having melt flow index 1.5 (ASTM method D 1238-70 at 190° using 2.16 kg wt.) and d. 924.8 kg/m<sup>3</sup>.

## C. Plasdac Documentation

55436 D/31 A17 ICIL 10.01.80 IMPERIAL CHEM INDS LTD *EP -32-309 11.12.80-GB-039757 (+000882) (22.07.81) C08F-04/62 C08F-10 Olefin polymerisation catalyst component prepn. - by treating inert particles with organo magnesium cpd., halide and transition metal cpd.	A(2-A08, 4-G1A) 109
D/S: E(AT BE CH DE FR GB IT LI NL SE) Intermediate priority: 6.6.80 - GB - 018582 (A) Prodn. of a component of an olefin polymerisation catalyst comprises treating (a) inert, solid particles having reactive sites with (b) organo Mg cpd. or complex or mixt. of the organo Mg cpd. and an Al cpd., (c) H halide, B halide, halogen, inter halogen cpd. or halides of Gp IVB, VB or VIB elements and (d) transition metal (m) cpd. of formula M(Oa)(Rb)(X)n (where M is a Gp IVA, VA or VIA transition metal; X is halogen other than F; R is opt. subst. hydrocarbyl or gp. OR; R' is opt. subst. hydrocarbyl; n is 0 or number up to valency of M with the exception that when M is Ti, n is not 4; a is 0 or 1; b is 0 or number up to valency of M and 2a + b + n equals valency of M. A Lewis Base (V) may also be used in forming the catalyst component. (B) The Olefin polymerisation catalyst is also claimed comprising component (A) and an organo-metallic cpd. of a	Gp IIA metal or of Al or a complex of an organometallic cpd. of a Gp IA or IIA metal with an organo Al cpd. USE The catalyst is esp. used to polymerise ethylene opt. mixed with a different olefin such as butene-1 in the gas phase. DETAILS TiCl <sub>4</sub> may be used in the prepn. of (A) in an amt. such that not above 75 mole % of the total of transition metal cpds. present in the final product are derived from TiCl <sub>4</sub> . Pref. (a) is an oxide of a metal including Si of Gps I-IV (b) is a dihydrocarbyl Mg cpd. and (c) is a H halide, Si halide (R <sub>1</sub> ) <sub>2</sub> SiX <sub>2</sub> -g, hydrocarbyl halide of formula R <sub>1</sub> (X <sub>1</sub> g), (R <sub>1</sub> is H or hydrocarbyl; R <sub>2</sub> is obtd. by removing H atoms) from a hydrocarbon cpd.; X is as above: f is 1-3 and g is 1-10), P (oxy) halide, B halide, Cl or Br. Pref. (d) is V oxytrichloride, tetrakis (ethoxy) Ti, tetrakis (n-butoxy) Ti, bis(iso-propoxy) Ti dichloride, bis(n-butoxy) Ti dichloride, Zr tetrabenzyl or Zr tetraneophyl. EP - 32309-
In (A) all the components may be mixed in a single stage and pref. the components are added in sequence to component (a). The reaction product need not be separated after each stage or may be washed and separated prior to proceeding to the next stage. EXAMPLE The catalyst component (A) was prepd. by (i) reacting 72g alumina, 720cc isoparaffin fraction and 11.9 cc SiCl <sub>4</sub> , (ii) adding 55.7 cc of a 0.62 M soln. of Mg dibutyl in the isoparaffin fraction, (iii) adding 121 cc of a 0.24 M soln. of bis (isopropoxy) Ti dichloride in the isoparaffin fraction. Ethylene under 80 psi was polymerised using the above component to consume 1.0 - 1.5 kg/hr. and a 0.1 M soln. of Al triisobutyl in hexane added at a rate of 40 m mole/hr. The obtd. polyethylene had MFI of 31.2 (ASTM Method D 1238-70), density 923.4 Kg/m <sup>3</sup> . (45pp966). (E)ISR: No Citns.	

Figure 2. Abstract comparisons.

was not indexed, because it was deemed to be a common reactant for the type of reaction involved. CAS says it indexes the novel features of a patent, which seems to me a curious usurpation of the responsibility of the patent examiner. These indexing rules can lead to substantial information loss in searching and provide a strong argument for searchable abstracts in online CA files, since the information involved is often included in the abstract. Points such as these have been brought to the attention of CAS management, which has

responded by agreeing to reexamine the policies.

The Registry system is potentially superb in dealing with the compositions of copolymers. In practice, it is considerably less than that. The use of words rather than Registry Numbers to index most synthetic rubbers is one example, but at least if one understands the policy, he or she can use both words and numbers in the search strategy. I believe that it would be beneficial to users to have not only the Registry Numbers but also the names that they stand for as a searchable part

## A. Plasdac Alerting

DUPO \* A23 84-001219/01 \* EP -96-805-A  
 Oriented polyamide monofilaments of improved tensile modulus - after extended immersion periods in water, have vinylidene chloride copolymer coating  
 DU PONT DE NEMOURS CO 13.12.82-US-449498 (01.06.83-US-383455)  
 F01 P14 P24 (A14 A82 A94) (28.12.83) A01k-91 A46d-01 D06m-15/32  
 01.06.83 as 108428 (1616AP) (E) FR1574864 US2431056 1.Jnl.Ref E(DE FR GB IT)  
 Novel oriented polyamide monofilament is uniformly coated with 2-10 wt.% (on monofilament) of a vinylidene chloride ethylenically unsatd. comonomer contg. at least 75 wt.% vinylidene chloride units. Also claimed is the prepn. of a coated monofilament.  
 The copolymer is pref. vinylidene chloride-methyl methacrylate-itaconic acid terpolymer. The coating pref. also contains 1-5 wt.% (on solids) of a wax.  
 The monofilament has a wet-to-dry tensile modulus ratio of at least 0.6 after 16h immersion in water. This gives the filament uniform performance characteristics which make it esp. useful in fishlines of dia. 0.102-1.270mm, and as toothbrush bristle of dia. 0.152-0.356 mm. (15pp Dwg.No.0/2)  
 C84-000289

## C. Plasdac Documentation

84-001219/01 A23 F01 P14 P24 (A14 A82 DUPO 01.06.82  
 DU PONT DE NEMOURS CO \*EP -96-805-A  
 13.12.82-US-449498 (+US-383455) (28.12.83) A01k-91 A46d-01  
 D06m-15/32  
 Oriented polyamide monofilaments of improved tensile modulus - after extended immersion periods in water, have vinylidene chloride copolymer coating  
 C84-000289 D/S: DE FR GB IT.  
 Novel oriented polyamide monofilament is uniformly coated with 2-10 wt.% (on monofilament) of a vinylidene chloride-ethylenically unsatd. comonomer contg. at least 75 wt.% vinylidene chloride units.  
 Also claimed is the prepn. of a coated monofilament.  
**ADVANTAGE/USES**  
 The monofilament has a wet-to-dry tensile modulus ratio of at least 0.6 after 16 h immersion in water. This gives the filament uniform performance characteristics which make it esp. useful in fishlines of dia. 0.102-1.270 mm., and as toothbrush bristle of dia. 0.152-0.356 mm.  
**COATING**  
 The copolymer is pref. vinylidene chloride-Me methacrylate-itaconic acid terpolymer.  
 The coating pref. also contains 1-5 wt.% (on solids) of a

Immersion time (hr)	Tensile Modulus (MPa)	Tensile Strength (MPa)	% Elongation at break	% Elongation at 1/4 break load
0	1182	629	27.0	10.6
2	1179	618	31.9	11.4
4	1071	680	36.2	11.7
6	1066	651	33.4	11.1
16	937	649	33.3	12.1

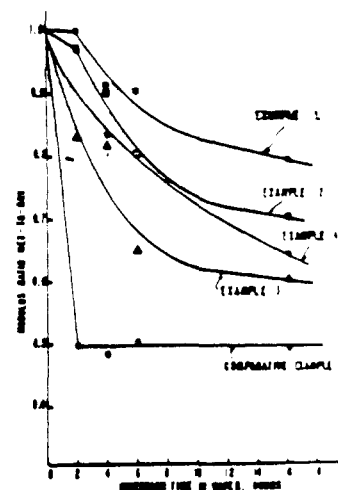
(15pp1616WADwgNo0/0).  
 (E) ISR: FR1574864 US2431056 1.Jnl.Ref.

## B. Chemical Abstracts

100:105040z Coated polyamide monofilament. Hansen, John Edward (du Pont de Nemours, E. I., and Co.) Eur. Pat. Appl. EP 96,805 (Cl. D06M15/32), 28 Dec 1983, US Appl. 383,455, 01 Jun 1982; 15 pp. Oriented polyamide monofilaments uniformly coated with 2-10% copolymer contg. ~75% vinylidene chloride are useful as com. fishing lines. Thus, a 1:8.5:90.5 itaconic acid-Me methacrylate-vinylidene chloride copolymer [27379-75-5] was coated on an oriented, 0.432-mm nylon monofilament. The wet-dry tensile modulus ratio after 2 h in water was ~1:1, compared with ~1:2 without the coating.

A(4-E7, 5-F1E1, 11-85A, 12-F1, 12-V4) F(1-D3, 1-E, 1-H6, 4-G) 1:5  
 wax.  
**PREPARATION**  
 The monofilament is dipped into an aq. emulsion comprising 10-50 wt.% vinylidene chloride copolymer with 1-5 wt.% (on copolymer) of a wax.  
 The filament is pref. passed through an aq. bath maintained at an elevated temp. prior to dipping in the emulsion.  
**EXAMPLE**  
 Oriented nylon monofilament of 0.432-0.330 mm. dia. was passed through a water bath at 100°C for 8.3 secs. and 450g tension and primed with a 5 wt.% (solids) aq. soln. of Serfine 2012 (RTM) and dried.  
 This was then passed through a coating bath of 22 wt.% solids aq. copolymer emulsion contg. 1.5 wt.% Na lauryl sulphate dispersant and 2 wt.% carnauba wax.  
 The copolymer was 90.5/ 8.5/1.0 vinylidene chloride/ Me methacrylate/itaconic acid.  
 The dried filament was tested according to US3595952 after initial conditioning for ≥48 hr. at 50% RH and 73°F and opt. immersion in water.  
 The results were:

EP-96805-A+



EP-96805-A

Figure 3. Abstract comparisons.

of the indexing record in all of the online CA files. This would be particularly helpful in generic searches.

An area in which I think CAS has missed the boat is that of copolymers with specialized structures, especially graft and block copolymers. Block copolymers have properties very different from those of random copolymers and deserve their own Registry Numbers. Graft copolymers are likewise different and should be identified uniquely on the basis of the

composition of the backbone and that of the grafting monomers. Yet CAS policy to date is to assign a single Registry Number for a given collection of comonomers, regardless of the structure. I believe that the CAS system has more inherent capability to register copolymer systems distinctly than any other available system, since none of the others is geared to the open-ended assignment of a unique term for each structurally distinct polymer entity.

- Controlled Index Terms
  - Substances (Registry Numbers)
  - Structure, Substructure (Registry, DARC, Dictionary files)
  - General Terms
- Text Modification, Uncontrolled Language
  - Linkable to Index Term in Most Online Files
- Title Words
- Uncontrolled Keywords from CA Issue Indexes
- Patent Classification
- CA Section Headings

Figure 4. Subject-access points in *Chemical Abstracts*.

Subject: Titanium-vanadium polymerization catalysts

Strategy: POLYMERIZATION CATALYSTS/IT (L) (:TITANIUM OR :TITANATE) (L)  
(:VANADIUM OR :VANADATE OR VANADYL)

Hits: ... Polymerization catalysts: (magnesium titanium vanadium  
chloride ...0

Strategy: POLYMERIZATION CATALYSTS/IT AND (:TITANIUM OR :TITANATE) AND  
(:VANADIUM OR :VANADATE OR VANADYL)

Noise: Polymerization catalysts: (aluminum fluoride compd.-titanium  
compd., for ethylene)  
7705-07-9, uses and misc: (catalysts, contg. aluminum chloride  
and vanadium chloride, for polymn. of ethylene)

Figure 5. Linking to avoid retrieval noise.

A far tougher nut to crack is the situation in which polymer differences are the result of differences in molecular weight, or microstructure, or incremental differences in comonomer composition. One can generate quite a list of different polymers by varying all of these values for the simple combination of ethylene and propylene; any attempt at unique registration would undoubtedly lead to chaos. One possible compromise might be to assign some sort of data tag for composition ranges, perhaps for extreme molecular weight values, at least for the most common commercial polymer systems. In a sense, tags of this sort would parallel the subdivision of index entries for common chemicals in *CA* and could help greatly in leading the user through reams of information. *CAS* is currently reexamining indexing policy in this area, and I look forward to significant advances in the future. But is there anything that can be done about the inadequate indexing of the past?

Another problem that I have found in the assignment of Registry Numbers to graft copolymers has been an apparent lack of consistency. Figure 6 illustrates the situation, covering some 14 references from the 1977–1981 period, all dealing with styrene–diene backbones that have been grafted or maleinized and, in some instances, postreacted after grafting. In this small set six different situations pertained; a situation I consider to be totally unacceptable. I am told that a recent meeting of *CAS*'s North American Users' Council did not consider the situation to be a serious one. I differ, emphatically. We need consistency in registration, and I suspect that the most useful system would be one in which grafted copolymers are registered before any postreaction. In the meantime, the user should be alerted to try every possible combination of words and Registry Numbers for monomers, intermediate polymers, and final product, using links to eliminate things that are out of context.

Before leaving copolymer registration I would like to tip my hat to the superb job that *DIALOG* has done in allowing us to search its Registry dictionary files by registered components—the Registry Numbers for each individual mo-

- No RN for polymer system
- RN for each specific backbone or graft monomer (one grafting monomer was non-specific)
- RN for backbone pre-grafting
- RN for grafted polymer (where no post-reaction takes place)
- RN for grafted polymer before post-reaction
- RN for grafted polymer after post-reaction

Figure 6. Inconsistency in indexing graft copolymers.

- Plasdoc code
  - Originally punch card-based
  - Limited number of terms available without radical revision
- Derwent chemical code
  - If patent also in Chemdoc
- Manual codes
  - Plasdoc, other CPI and EPI sections
- Words from augmented titles
- Abstract words
  - 1970+ at present
- International patent classes
- U.S. patent classes
  - Indirectly, by crossfile from USCLASS, US Patents
- Derwent classes
- Individual substance registration
  - About 2,000 Chemdoc registry substances, plus 750 Plasdoc registry substances, 1984+

Figure 7. *Plasdoc* subject-access points.

nomer involved in a copolymer system. This is extremely simple to do and far more precise than previous methods based on combination of molecular formulas and/or nomenclature.

#### RETRIEVAL: PLASDOC

Let us look now at the retrieval capabilities of *Plasdoc*, outlined in Figure 7. The primary means of searching is the *Plasdoc* code, derived from a punch card based system originally developed by ICI Plastics and enhanced several times over the course of *Plasdoc*'s existence. A number of other searchable parameters are available, including coding terms from other sections of the overall Derwent database when patents appear in those sections as well as in *Plasdoc*. Each of the additional access points can be very helpful. For the first time in 1984 we have been able to search for specific compounds in *Plasdoc*, not only some 2000 relatively common substances added to the *Chemdoc* retrieval system in 1981 but an additional 750 substances that are often used in polymer systems. Abstract words have been especially useful since 1981 for pinpointing concepts handled inadequately by the *Plasdoc* code, and the recent addition of abstracts from 1970–1980 to the file has been a significant improvement in file capability. It seems likely that abstracts from 1966–1969 will be added in the near future.

The scope of the *Plasdoc* code is illustrated in Figure 8, and it looks quite similar to Figure 1, which outlined the scope of polymer information. Its breadth is fine; the problem has always been lack of depth, lack of specificity. The number of terms originally available was limited by the number of punch positions on a standard 80-column card, although the pairing of punch positions did allow some expansion of the limit—with some attendant noise from false coordinations. Noise was not a big problem in the early days; one fed a card sorter with stacks of cards that were imprinted with those excellent Derwent documentation abstracts. One obtained a modest-sized hit stack and scanned through the abstracts.

With the size of today's file, though, and with online output that may provide titles or alerting abstracts but not docu-

- A. General and multifacet terms; novelty descriptors
- B. Olefinic monomers and their addition polymers
- C. Condensants and their polymers
- D. Natural polymers and their derivatives
- E. Modified polymers
- F. Catalysts and controllers
- G. Polymerization processes
- H. Reaction processes (excluding polymerization)
- J. Additives or materials associated with polymers
- K. Plant and laboratory operations
- L. Shaping and finishing of polymers
- M. Form or shape of polymers
- N. Properties
- P. Uses of polymers

Figure 8. Scope of *Plasdoc* code.

**MONOMERS:** Specific Hydrocarbon Mono- and Diolefin Monomers Searchable in *Plasdoc*

Ethylene	Styrene	Butadiene
Propylene	Vinyltoluene	Isoprene
Butene-1	$\alpha$ -Methylstyrene	Divinylbenzene
Isobutylene		Piperylene (1982)
4-Methylpentene-1		

All others fall in catchall categories -- including such important monomers as Hexene-1; dicyclopentadiene; ethylidenenorbornene; 1,4-hexadiene; etc.

**CATALYSTS:** Ziegler Catalyst Components

- Transition metals and their compounds
- Halides, Oxyhalides
  - Titanium halides, oxyhalides
  - Titanium trivalent halides
  - Other titanium halides, oxyhalides
  - Other halides, oxyhalides
- Oxides
- Other transition metals and compounds

Until 1977, this is all that was available for searching the transition metal component of Ziegler catalysts. In 1977 terms were added to identify transition metals other than titanium. Finally, the start of compound registration in 1984 permits the identification of the more common specific catalyst components.

Figure 9. Low specificity in *Plasdoc* code.

mentation abstracts, the lack of specificity becomes a substantial problem. Large numbers of hits are often produced, and usually one must then obtain the documentation abstracts to check them out. The less specificity available in searching, the more references that must be checked. To get an idea of the lack of specificity, consider the fact that until 1984 one could not search for specific plasticizers, or antioxidants, or catalyst modifiers, or etc., unless they were deemed to be novel and thus coded in *Chemdoc*. In searching for maleinization one has had to consider all references on polymer alkylation, because Derwent treats maleinization as alkylation rather than grafting. Grafting monomers are coded; alkylating agents are not. In searching for matte-finished films one must search for gloss, since a single term is used to describe a property and its opposite. Figure 9 shows the sparseness of terms available to describe hydrocarbon monomers and the transition metal components of polymerization catalysts.

I have referred earlier to the value of linking logic in minimizing noise. *Plasdoc* does have the capability of linking indexing terms in subrecords and in recent years has made more use of multiple subrecords to separate ideas that should be separated. But there are inherent problems—especially in the first dozen years of the file. Thus, Figure 10 shows that the scrambling of monomer terms in polymer blend systems leads to considerable ambiguity regarding what system is actually present. In 1978 some precoordination was introduced

ETHYLENE + VINYL CHLORIDE + VINYL ACETATE + HOMOPOLYMER + COPOLYMER

PE + VC-VAc ?

PVC + E-VAc ?

PVAc + E-VC ?

Figure 10. Term scrambling without precoordination.

SEARCH FOR: Ethylene-Ethyl Acrylate-Methyl Methacrylate Terpolymer

CAS Registry No. 26812-69-1

CA Postings, 1967-date: 0

Plasdoc Strategy(1) Ethylene terpolymer AND Ethyl acrylate terpolymer<sup>®</sup> AND Methyl methacrylate terpolymer<sup>®</sup> (113 hits)

(2) Ethylene(L)Acrylic ester(L)Methacrylic ester(L)Methyl(L)Ethyl(L)Terpolymer (294 hits)

(3) 1 AND 2 (105 hits)

Notes

- Run on WPIL file, 1981 through Week 8413, but terms labeled <sup>®</sup> available only since 1982.
- Precoordinated terms in Set 1 useable only with AND logic, not LINK, so that set was ANDed with set 2 to give result in which all monomers coded in same polymer system.
- Set 2 represents the system capability before introduction of pre-coordination in 1978.

Figure 11. Copolymer ambiguity even with some precoordination: the ghost of Markush.

to the system, enabling one to determine whether a given monomer was present as a homopolymer, binary copolymer, or ternary or higher copolymer. Then, in 1982, additional precoordination was introduced, making several dozen common copolymer systems directly searchable as bound terms.

One might think that this had solved the problem, at least for common systems. Figure 11 shows that the amount of noise has been decreased but, where there is not a bound term in the system for the specific copolymer of interest, the amount of noise is still uncomfortably large. We see here a substantial number of "hits"—50 per year with the help of precoordination, nearly 100 per year without it, for a polymer system that seems not to have been reported once over a period of nearly 20 years. Some of these patents may well permit the terpolymer of E-EA-MMA as an option; others may be higher polymers including ethylene, ethyl acrylate, methyl methacrylate, and additional monomer(s).

However, the bulk of the references involve polymers comprising ethylene, an acrylic or methacrylic ester, and one or more additional monomers. This sort of retrieval noise is similar to that obtained in the searching of Markush (generic) chemical formulations, in which groups present *only as alternatives* are retrieved by AND logic, as if both were present.

For the record, the IFI/Plenum files produced results similar to those found in *Plasdoc*. For the period of 1971–1981, *CLAIMS-Uniterm* produced 203 references, *CLAIMS-CDB* with superior specificity capabilities, 124. Again, nearly all of these involved systems including ethylene, an acrylic or methacrylic ester, and some additional monomer(s).

CA's capability of indexing only specific systems cannot cope with the options produced by patent claims. Existing generic systems, on the other hand, are too noisy. Something better must be possible. It is necessary to develop some system for Markush searching that is capable of distinguishing a situation in which two groups are both present from one in which either of the two is present, but not both. It is similarly necessary to do the same regarding comonomers in copolymers. In the meantime, it is advantageous for a generic system to include as many bound copolymer terms as possible. *CLAIMS* is clearly ahead of *Plasdoc* here.

I would certainly like to see *Plasdoc*'s list of bound terms increase; now that punch card limitations are gone, there is no reason for omitting any reasonably common system from the indexing vocabulary. More bound terms, the searchability

- General Index terms
  - some with roles (present, reactant, product)
  - numerous bound polymer terms
  - polymer class terms
- Compound terms
  - all with roles
  - associated compound registry file for compound identification
- Fragment terms
  - for generics, uncommon compounds
  - all with roles
  - linking of fragments for given substance
- Patent classification
  - all U.S.; also IPC
- Title, abstract and/or representative claim words
- CAS Registry numbers, 1967-79
- Special system of polymer roles

**Figure 12.** Access points in *CLAIMS-CDB*.

since 1984 of some 2000 *Chemdoc* and 750 *Plasdoc* registry compounds, and the availability of searchable abstracts in back-files should help improve retrieval in the future. One possibility for helping us cope with noise is a system that Derwent is investigating, which could provide copies of basic abstracts as offline search output. It remains to be seen whether such a system will be technically and economically feasible, but the prospect is intriguing.

There is another extremely important *Plasdoc* searching capability that must be mentioned: manual code cards. Manual codes, essentially key concepts, are used to define sets of cards containing documentation abstracts. Scanning these cards is still the best way of searching some types of technology. For example, it is about the only way of carrying out most searches for catalyst systems, given the low indexing specificity illustrated in Figure 9. Some of the manual code card sets are uncomfortably large, and I have always felt that Derwent assigns fewer manual codes than it might, which makes some code sections less complete than they should be. Nevertheless, manual code card searching, old-fashioned though it may be, is still an extremely valuable adjunct of *Plasdoc*.

#### RETRIEVAL: IFI FILES

IFI/Plenum's *CLAIMS-Uniterm* file does have some special polymer capability, since there are a number of specific indexing terms for homopolymers and bound copolymer systems, and polymers that do not have their own terms can be searched for by using the appropriate terms for the monomers along with general terms for the type of polymer. *Uniterm*'s extensive controlled vocabulary is open-ended, so that new indexing terms are added to the system as they become needed. But the system that I want to discuss in more detail is the *CLAIMS-CDB* file, available only to subscribers, because this file has some of the most unique and valuable indexing capabilities around today.

Subject-access points in the *CDB* are shown in Figure 12. If I have passed quickly over the retrieval systems of CA and *Plasdoc*, at least those databases have a broader user community, so that many information users are undoubtedly familiar with them. *CDB*, with access limited to a smaller group of subscribers, is both less familiar and highly complex. There is no way to do justice to its system within the space available here. A *CDB* description appears in the proceedings of a recent conference on generic structure searching and provides

**Table II.** Roles in *CLAIMS-CDB* System

	present	reactant	product
compounds, general terms, fragments	10	20	30
alloys, glasses, etc.	40	50	60
polycarbons, homo/co	41, 71	51, 81	61, 91
polycarbons, mod, homo/co	14, 17	15, 18	16, 19
polyethers, homo/co	42, 72	52, 82	62, 92
polyesters, homo/co	43, 73	53, 83	63, 93
polycarbonates, homo/co	44, 74	54, 84	64, 94
polyamides, homo/co	45, 75	55, 85	65, 95
polyurethanes, homo/co	46, 76	56, 86	66, 96
polysiloxanes, homo/co	47, 77	57, 87	67, 97
other regular polymers	70	80	90
unusual polymers	12	22	32
modified polymers (excluding polycarbons)	11	21	31

**Table III.** Roles for Ethylene, 1982 to September 1983<sup>a</sup>

	present	reactant	product
ethylene	92	442	88
in polycarbon homopol	849	83	200
in polycarbon copol	770	112	203
in mod polycarbon homopol	238	23	103
in mod polycarbon copol	330	37	203
14 other roles	15		14

<sup>a</sup> Total postings, file 925: 2123.

**Table IV.** Indexing of Chlorinated Polyethylene

	role	
ethylene	14	present, mod homopolycarbon
chlorine	14	modifier in homopolycarbon
olefin homopolymers/acyclic	11	modified
chlorinated polyethylene	10	bound polymer term

some additional detail, but even there the treatment is necessarily brief.<sup>2</sup>

Keys to the *CDB* system are the following: specific descriptors for many relatively common chemicals, including chemicals involved in polymers; a system of fragments and links to describe generic and uncommon compounds; and a system of roles. For simple chemicals, the roles are the traditional ones: present, reactant, product. For polymers, there is a highly developed role system that conveys a great deal of information about not only the monomers incorporated into polymers but even chemicals used to modify them.

The complete *CDB* role system is shown in Table II. Table III shows how the system of roles provides an enormous amount of discrimination in describing references concerning ethylene, over a 21-month period. Of the over 2000 references, 92 cover instances where monomeric ethylene is present, 442 in which it is a reactant, and 88 in which it is produced; 200 cover the preparation of ethylene homopolymers and 203 the preparation of modified ethylene copolymers; in 770 references ethylene is present in unmodified polycarbon copolymers. In all, ethylene appears in 29 different roles during this brief period; the system has given us a lot of information.

Table IV shows how the system of roles extends not only to monomers but also to chemical modifiers, with the chlorine in chlorinated polyethylene getting the role for modified homopolycarbons. It would have the role for polyethers in a chlorinated polyether and for polyamides in a chlorinated polyamide. Similar polymer roles are assigned to hydrogen in hydrogenated polymers, to oxygen in oxidized ones, and to cross-linkers in vulcanized rubber.

In discussing CA, I noted the Registry system's potential for distinguishing block and graft copolymers. *CLAIMS-CDB* can actually do some of this, since the backbone polymer in a patent on grafting will get the role of reactant, while the final grafted polymer gets the role of product. This only pertains, however, in patents that actually cover the grafting operation.







- Registration of polymers with regard to structure; more consistency in registration (CA)
- More complete indexing of essential components; closer attention to claims; handling of generics (CA)
- Fuller description of scope of patent (CA abstracts)
- Searchable abstracts (CA)
- More indexing terms, especially bound copolymers, catalyst components (Plasdoc)
- Generic systems that distinguish between components that are alternatives, and those that must both be present.
- More attention to process details and equipment
- More use of linking logic

Figure 15. Some desired database improvements.

develops the Registry to the point where it deals with special polymer structures such as blocks and grafts and gets rid of indexing policies that omit important ingredients from the indexing. I hope, too, that they can develop a system to deal with generics and have their abstracts show more fully what the scope of a patent is. CA really needs searchable abstracts—and the searchable abstracts should be available not only on STN but on DIALOG, SDC, and other hosts.

I hope that *Plasdoc* will add more indexing terms beyond those added recently, especially terms to describe bound copolymers and catalyst components. I think that we desperately

need generic systems that can distinguish components that are present together from those that are alternatives. Otherwise, file growth will further magnify the noise that is often intolerable even today.

I would certainly like to see more attention paid to process details and equipment, something that *Plasdoc* probably does best today. I want to be able to know with certainty when polymerization was run in a tubular reactor and when it was run in gas phase. And I would give a great deal for a system that could tell me with assurance that a patent really involved grafting in an extruder, rather than just the extrusion of a grafted polymer.

Finally, I would like to see an extension of linking logic, one of the best ways of cutting down on noise. There is certainly room for linking of nonfragment terms in *CLAIMS-CDB* and of the new key serial and registry terms in *Plasdoc*. Others could surely add to the list. I look forward to future enhancements of today's invaluable services.

## REFERENCES AND NOTES

- (1) POST-P and POST-J are no longer published, but they served as a pilot development that led to improvements in CA's polymer coverage.
- (2) Kaback, S. M. "The IFI/Plenum Chemical Indexing Systems". "Computer Handling of Generic Chemical Structures"; Barnard, J. M., Ed.; Gower: Aldershot, Hampshire, England, 1984; pp 49-65.

## The Paradox of Patentability Searching<sup>†</sup>

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Patentability searching is, by its nature, a paradox. To be patentable, a new product or process must never have been described or suggested in the prior art. The searcher charged with confirming the patentability of an invention is thus presented with three dilemmas: how to design an exhaustive search for a reference that is believed not to exist, how to recognize a reference describing the invention in a different context or vocabulary, and, if no relevant references are found, how to tell when the search is complete.

Most research and development in science and engineering is conducted for the purpose of making inventions, in the sense that any new product or procedure and any improvement in an existing product or procedure are inventions. Having invested large sums of money in its development, it is natural for the successful developers of a new product or process to wish to reserve for themselves the right to profit from their invention. The accepted way to prevent others from making, using, or selling an invention is by patenting it. But not every new product or process is patentable. In the U.S. and in most other countries, only an invention that is new, useful, and nonobvious can be granted a valid patent.

Applying for a patent on an unpatentable invention represents an unnecessary expense and an unnecessary risk. The patent offices of many countries publish patent applications before determining whether or not the invention being claimed satisfies the national standards of patentability. If a patent application claiming an unpatentable invention is filed in one of these countries, the unpatented technology disclosed in the published application is freely available for use by the public in that country and in every other country where patent protection has not been obtained. The developers may well wish

to maintain the details of the invention as a trade secret or to abandon the invention entirely so as to avoid sharing it with their competitors. It is possible to minimize the risk of public disclosure of an unpatentable invention by performing a patentability search before drafting the patent application.

For a hypothetical example, let us take the development of a new chemical compound by a Dr. Smith of the Panacea Cosmetic Co. Dr. Smith has had the new compound tested and knows that it prevents dandruff in rats. He has devised a new shampoo formulation that includes the new compounds and found that these compounds also reduce the incidence of dandruff, although not as well as the original compound. If possible, the Panacea Cosmetic Co. would like to patent Dr. Smith's whole genus of antidandruff agents, the method by which the compounds were synthesized, the shampoo formulation containing any of the compounds in the genus, and the method for preventing dandruff by shampooing with such a formulation, all of which would be patentable inventions under U.S. patent law if the standards of utility, novelty, and non-obviousness are met. Since it is an international company, Panacea intends to patent the invention in each of 20 countries. If it is unable to obtain such broad coverage, Panacea will settle for a patent that claims only the most active compound, and if the compound per se is not patentable, it will make do with a patent that protects only the shampoo formulation or the method of treating dandruff with it.

<sup>†</sup> Presented at the Herman Skolnik Award Symposium in honor of Montagu Hyams before the Division of Chemical Information, 188th National Meeting of the American Chemical Society, Philadelphia, PA, August 28, 1984.