# Condensation Polymer Information: Problems and Opportunities†

ROBERT N. WILKE and ROBERT E. BUNTROCK*

Amoco Corporation, F-1/IS, P.O. Box 3011, Naperville, Illinois 60566-7011

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Searching for information on addition polymers, although not trivial, is relatively straightforward. However, the involvement of functional groups makes searching for information on condensation polymers considerably more difficult. Current methods of searching for condensation polymers will be discussed along with suggestions for improvement. Problem areas include precise definition of functional groups and polymer products, indexing of several compositions in the same record (coincidence, mixtures, blends), and stereochemistry. The online files and indexing systems discussed include Chemical Abstracts, Derwent WPI, and IFI CLAIMS.

## INTRODUCTION

Searching for information on condensation polymers is inherently more difficult than searching for information on addition polymers. (For typical addition polymers, the molecular formula of the repeating unit is the same as that of the monomer, and the total molecular weight is the sum of all of the monomer units. Typically, unsaturated groups are linked in addition polymerization. For a typical condensation polymer, there are fewer atoms in the repeating unit than in the monomers. The atoms lost in condensation polymerization are typically part of small molecules such as water, ammonia, hydrogen sulfide, etc.)

Whereas many addition polymers are homopolymers, condensation polymers for the most part have at least two reactants to deal with for each polymer. However, this does not imply that addition polymer searching is easy. There can be many difficulties in identifying the polymer, defining stereochemistry, or linking the right monomers with the right polymer in multicomponent mixtures or blends. An example of one of these is the problem of identifying which monomer is used to make a polybutene.[1] Was it 1-butene, 2-butene, or a mixture? However, with addition polymers, there is usually less of a problem to define or index the structure of a monomer, if that monomer is identified.

Searching for polymer information is a difficult proposition with all of the major patent information databases. For this study, only these databases have been considered: Chemical Abstracts Files (both the CA and the Registry Files), Derwent's WPI Files and the IFI Claims Comprehensive Database. The CAS files were searched on STN; IFI and WPI files were searched on DIALOG. As can be seen in other papers in the symposium,[2] database producers have described plans for improving polymer indexing in the future. However, our work describes current and past practice and is intended to show the need for future improvements.

The main problems today in searching for any polymer information are inadequate conceptual linking of index terms and inadequate structure definition. Inadequate linking may involve the failure to link monomers or condensates to form polymers or copolymers, the failure to link polymers to form blends, and the nonlinking of polymers with other structural or nonstructural information. Inadequate definition of structural information may be represented by use of generic definitions of either a monomer or structural repeating unit (SRU) instead of actually defining the structures.

To illustrate the present linking systems used by the major patent information databases to index polymers, three different areas of polymer searching will be described: polymer stereochemistry, polymer blends, and polymerizations that form structures not related to their starting materials, such as those polymerizations involving ring opening or ring closing. These areas will also be limited to condensation polymers, except for stereochemical topics which apply mainly to addition polymers.

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## CONDENSATION POLYMERS: DEFINITION OF STRUCTURE

This work is focused on condensation polymers because of additional problems in both definition and searching due to the involvement of functional groups. Polymerization paths and products of many functional groups may vary with changes in reaction conditions. Therefore, the structure of condensation polymers is determined not only by the functional groups but also by the reaction conditions. For several types of functional groups, it is necessary but not sufficient to describe resulting polymers as "polymers of ..." (the given monomers). Additional polymeric structural information needs to be given.

A good example of multiple reactions of monomer functional groups are isocyanates. Isocyanates can homopolymerize to give nylon 1 polymers. This reaction takes place by addition across the C=N bond (Figure 1). Isocyanates can also undergo addition reactions and polymerizations with olefins or compounds containing a C=C bond (Figure 2). Diisocyanates are also used to form condensation polymers. The most widely used of these reactions is the reaction of diisocyanates with polyols to produce polyurethanes or with dicarboxylic acids to produce polyamides (Figure 3). Isocyanates can also undergo addition–condensation reactions to produce some unique polymeric systems. For example (Figure 4), reaction of diisocyanates with hydrogen cyanide can produce cyanoformamidines which can cyclize to give polyiminoimidazolidinones. These can be hydrolyzed to polyparabanic acids.

## RING OPENING AND CLOSING

For condensation polymers as described in patents, often only the final polymer is identified. The starting monomers are not always identified, and even if the structure can be determined by inspection, it probably will not be indexed. This makes searching especially difficult in the Derwent and IFI Databases, where polymer indexing is based primarily on the starting monomers. This is especially true when the polymerization reaction involves a ring opening or closing, or some other major structural change to one or more of the monomers.

An example of this type of reaction is the preparation of polythiadiazoles. These polymers can be formed from the reaction of a dithiohydrazide with a diacid chloride to give a polythiohydrazide, which can be dehydrated to a polythiadiazole, or by the reaction of a dihydrazide with a diisothiocyanate followed by dehydration (Figure 5). Similar types

0095-2338/91/1631-0463$02.50/0 

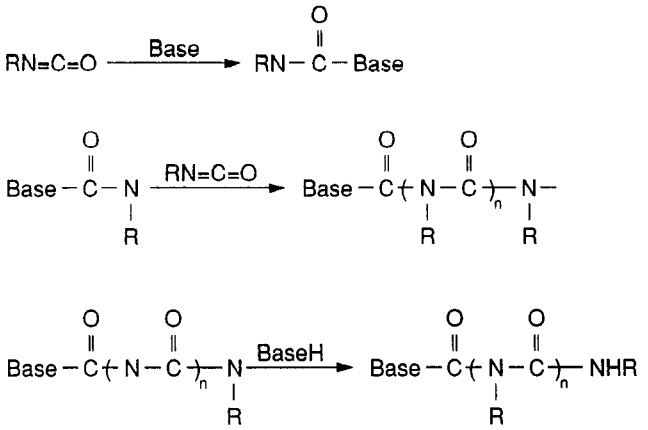

Figure 1. Homopolymerization of isocyanates.

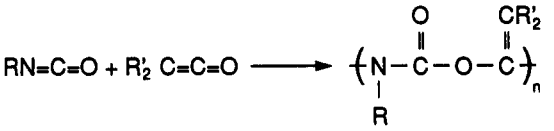

Figure 2. Addition reactions of isocyanates.

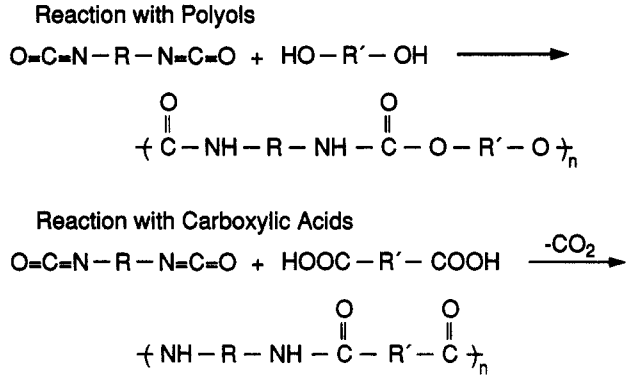

Figure 3. Isocyanates as condensants.

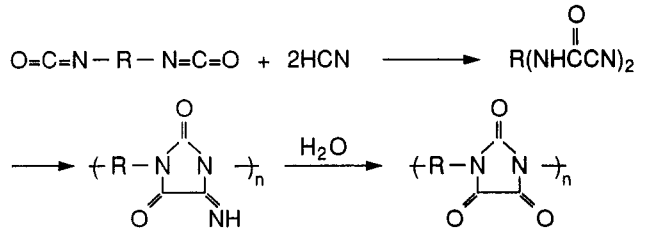

Figure 4. Addition–condensation reactions of isocyanates.

of reactions can be used to make polyoxadiazoles.

An example of a ring-opening reaction is the reaction of β-propiolactone with anions, where different anions can give different results. Reaction with an alkoxide proceeds by cleavage of the acyl–oxygen bond; reaction with sodium acetate proceeds by cleavage of the carbon–oxygen bond (Figure 6).

Another example involves both a ring-opening reaction and a subsequent cyclization reaction. This is the reaction of alkylene bisazlactones with diamines to give polyamides which undergo dehydration to give a polyimidazolinones (Figure 7).

Results of analysis of this reaction will show the differences in indexing between CAS, Derwent, and IFI. An example of Derwent WPI indexing will be described first. An abridged version of U.S. 4667012 is shown in Figure 8 (patent family EP 185493/JP 61143432/U.S. 4667012/U.S. 4785070).

From this record it can be seen that Derwent has indexed these polyimidazolinones as "condensation polymers; other

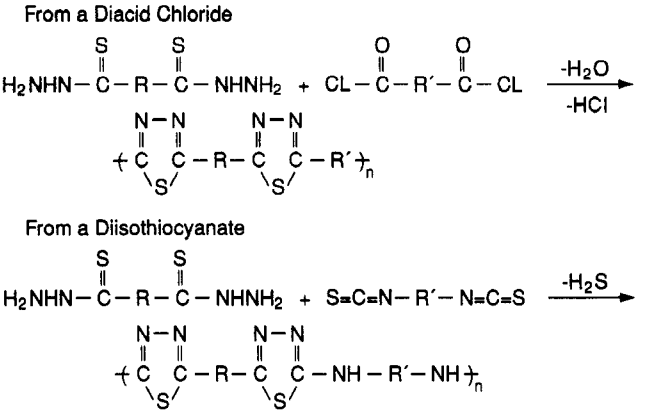

Figure 5. Preparation of polythiadiazoles.

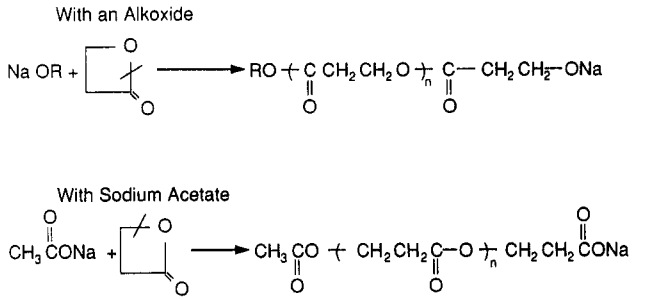

Figure 6. Reaction of β-propiolactone with anions.

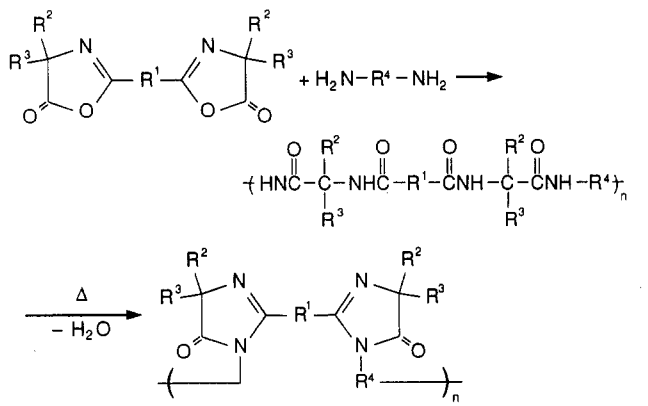

Figure 7. Reaction of bisazlactones with diamines.

Patent Family: EP 185493 JP 61143432 US 4667012 US 4785070

Polymer Fragment Codes

*101* 014 02& 028 035 038 039 041 046 05 06- 062 066 07- 072 074 075 08& 08- 080 081 086 09& 09- 094 10& 10- 116 141 143 147 149 15& 150 151 153 155 156 157 162 163 169 17& 170 175 185 191 192 195 196 197 206 207 208 209 225 229 231 239 24& 250 262 263 27- 273 277 292 293 31- 316 331 334 336 344 346 348 355 357 359 38- 398 402 405 417 419 440 442 477 512 516 518 521 532 537 54& 54- 541 546 55& 551 556 56& 560 566 57- 575 583 589 603 604 608 61- 642 657 678 684 688 689 720 724 725 726

Figure 8. WPI indexing, polymer fragment codes.

types (Plasdoc codes 153 + 720)", which is not very specific. Examination of the indexing shows it was also indexed to various diamines (206), and to "mixed group condensants, others, heterocyclic (197 + 175)", to lactams (192), or to lactones (195). The intermediate polyamides (141) were also indexed. In fact it could be indexed to many different condensants. This wide range of indexing means this record would be retrieved with a search strategy that had nothing to do with azlactones or imidazolinones. The most precise search would be to use text terms.

The IFI indexing for this patent (U.S. 4785070) is shown in Figure 9. The generic terms for the intermediate polyamide

General Terms:

POLYAMIDES, 10 11 20 21 30 31; POLYAMINES, 10 20 30;
POLYDIMETHYLSILOXANE, 10 20 30; POLYESTERS, 11 20 30 31;
POLYETHERS, 11 20 21 30 31; POLYIMIDAZOLES, 10 30;
POLYLACTAMS, 10 20 30; POLYLACTONES, 10 20 30;
POLYMERS/SPECIFIC/, 10 30; POLYSILOXANES, 11 20 30 31;
POLYUREAS, 10 20 30; POLYURETHANES, 10 20 30;
METALS/NOT SPECIFIC/, 20 90; AMINES AND SALTS, 20 70 80 90;

**Figure 9.** IFI indexing of imidazolinone patent, U.S. 4785070.

Fragment Terms:

CARBOCYLIC RING -- F CHNO SECONDARY CARBOXYLIC AMIDE FG (P-1)
F C2NO2 O=C-O-C=N (P-1) -- F C2NO2 0=C-O-C=N (P-2+)
F C2N2O O=C-N-C=N (P-1) -- F H2N PRIMARY AMINE FG (P-1)
HETEROCYCLIC RING -- HETEROCYCLIC RING (M) -- NITROGEN IN RING (M)
OXYGEN IN RING (M) -- PARTIAL RING UNSATURATION (M)
R I C3NO OXAZOLE RING (P) -- R I C5 CYCLOPENTANE RING (P)
R I C6 BENZENE RING (P) -- R II C3NOC5 GENERIC RING
R II C3NOC6 GENERIC RING

**Figure 10.** Imidazolinones, U.S. 4785070, oxazole IFI fragment terms.

Fragment Terms:

CARBOCYCLIC RING -- F CHNO SECONDARY CARBOXYLIC AMIDE FG (P-2+)
F CN C*N (P-2+) -- F CNO2 CARBAMIC ACID, CARBAMATE FG (P-2+)
F C2N2O O=C-N-C=N (P-2+) -- F HN SECONDARY AMINE FG (P-2+)
F N TERTIARY AMINE FG (P-2+) -- F NO2 NITRO FG (P-2+)
FUSED OR BRIDGED RING -- HETEROCYCLIC RING -- HETEROCYCLIC RING (M)
NITROGEN IN RING (M) -- PARTIAL RING UNSATURATION (M)
R I C3N2 IMIDAZOLE RING (P) -- R I C4 CYCLOBUTANE RING (P)
R I C5 CYCLOPENTANE RING (P) -- R I C6 BENZENE RING (P)
R II C6C6 NAPHTHALENE RING (P) -- RING UNITS, 4+ (M) Roles 12, 32

**Figure 11.** Imidazolinones, U.S. 4785070, polyimidazolinone IFI fragment terms.

TI Imidazolinone-containing polymers and copolymers

PI EP 185493

IT Cyclocondensation reaction
(of polyamides to polyimidazolinones)

IT Polyamides, preparation
(prepn. of, from bisazlactones, and cyclodehydration to polyimidazolinones)

IT Polymers, preparation
(imidazolinone group-contg., prepn. of, by cyclodehydration of polyamides formed from bisazlactones)

**Figure 12.** Imidazolinone Patent EP 185493, CA General Subject Indexing.

are indexed as well as the term polyimidazoles, which is used in place of polyimidazolinone. The starting azlactone is indexed as a substituted oxazole by the fragmentation codes as shown in Figure 10. These codes are only a portion of all the codes that are linked in the indexing. Finally, the polyimidazolinone products are indexed by the fragment terms shown in Figure 11.

Only part of all the indexing that is present in this record is shown. The fragment term record that is shown is the "polymer per se" indexing of the product polyimidazolinone. This ability of IFI to index "polymers per se" using the fragmentation codes allows them to adequately describe a polymer in terms of its structure even when it cannot be described in terms of its starting materials.

The Chemical Abstracts record for this patent exists for the equivalent European patent, EP 185493. In the first portion of this record the General Subject Index entries ("generic indexing") are shown (Figure 12). It involves the use of generic controlled vocabulary polymer terms linked with text modifiers.

IT 22102-60-9DP, polymers with adducts of Jeffamine CD-230 and 2-vinyl-4, 4-dimethyl-2-oxazolin-5-one 29513-26-6DP, Michael addn. products with Jeffamine CD-230, polymers with 3,3'-iminobispropylamine 104859-97-4P 104859-98-5P 104867-76-7 ....
(prepn. and dehydrocyclization of, to polyimidazolinones)

IT 104867-77-8P 104867-82-5P ....
(prepn. of, by cyclodehydration of polyamides formed from bisazlactones)

**Figure 13.** Imidazolinone Patent EP 185493, CA polymer indexing.

RN 22102-60-9
CN 5(4H)-Oxazolone, 2,2'-(1,4-phenylene)bis[4-methyl-

RN 29513-26-6
CN 5(4H)-Oxazolone, 2-ethenyl-4, 4-dimethyl-

**Figure 14.** Imidazolinone Patent EP 185493, registry monomer indexing.

RN 104859-97-4
CN 5(4H)-Oxazolone,
2,2'-[oxybis(2,1-ethanediylthio-2, 1-ethanediyl)]bis[4,4-dimethyl-,
polymer with N,N'-bis(2-aminoethyl)-1,2-ethanediamine

CM 1
CRN 89342-97-2
CN 5(4H)-Oxazolone,
2,2'-[oxybis(2,1-ethanediylthio-2,1-ethanediyl)]bis[4,4-dimethyl-,

CM 2
CRN 112-24-3
CN N,N'-bis(2-aminoethyl)-1,2-ethanediamine

RN 104867-76-7
CN Poly[imino(1,1-dimethyl-2-oxo-1,2-ethanediyl)imino-1,2-ethanediylimino-1,2-ethanediylimino-1,2-ethanediylimino-(2,2-dimethyl-1-oxo-1,2-ethanediyl)imino(1,6-dioxo-1,6-hexanediyl)]

**Figure 15.** Imidazolinone Patent EP 185493, registry polymer indexing.

RN 104867-82-5
CN
Poly[(4,5-dihydro-4,4-dimethyl-5-oxo-1H-imidazole-2,1-diyl)-1,4-phenylene(4,5-dihydro-4,4-dimethyl-5-oxo-1H-imidazole-1,2-diyl)-1,4-butanediyl]

RN 104867-77-8
CN
Poly[(4,5-dihydro-4,4-dimethyl-5-oxo-1H-imidazole-1,2-diyl)-1,4-butanediyl(4,5-dihydro-4,4-dimethyl-5-oxo-1H-imidazole-2,1-diyl)-1,2-ethanediylimino-1,2-ethanediylimino-1,2-ethanediyl]

**Figure 16.** Imidazolinone Patent EP 185493, registry polymer indexing.

In Figure 13 is shown the registry numbers for the azlactone monomers linked to text modifiers. The indexing also includes the registered SRU's for the intermediate polyamides and final polyimidazolinones.

As shown in Figure 14, CAS has indexed the starting azlactones as oxazoles. Some of the intermediate polyamides are indexed from their components, and some are indexed as SRU's (Figure 15). These polyamides are formed from the reaction of the oxazoles with 3,3'-iminobispropylamine. The product polyimidazolinones are indexed as SRU's (Figure 16).

## MIXTURES AND BLENDS

Mixtures and blends are particularly difficult to search. As luck would have it, they always seem to involve polymers that contain monomers from the same chemical classes. Some

S1 CT=ADIPIC ACID (S) RL=(45 OR 55 OR 65)

S2 CT=HEXAMETHYLENE DIAMINE (S) RL=(45 OR 55 OR 65)

S3 (S1 AND S2) AND CT=POLYHEXAMETHYLENE ADIPAMIDE (S) RL=(10 OR 20 OR 30)

S4 CT=PROPYLENE (S) RL=(41 OR 51 OR 61) OR CT=POLYPROPYLENE (S) RL=(10 OR 20 OR 30)

S5 CT=(MIXTURES OR BLENDS OR ALLOYS/POLYMERS OR COMPOSITES OR COMPOSITE/STO)

S6 S3 AND S4 AND S5

**Figure 17.** IFI strategy for blends search: polypropylene with nylon 66.

General Terms:
BLENDS; POLYAMIDES, 10 11 31; POLYESTERS, 11 31; POLYHEXAMETHYLENE ADIPAMIDE, 10 30; POLYHEXAMETHYLENE SEBACAMIDE, 10 30; POLYPROPYLENE, 10;

Compound Terms:
ADIPIC ACID, 43 45 63 65 75 95; HEXANE, 1,6-DIAMINO-, 45 65; HEXANEDIOL/1,6-/, 43 63; PIPERAZINE, 45 65; PROPYLENE, 41; XYLYLENEDIAMINE/M-/, 45 65; PHENYLENEDIAMINE/P-/, 45 65; TEREPHTHALIC ACID, 45 65 75 95; TOLUENESULFONIC ACID/P-/, 45 65; CYCLOHEXANEDICARBOXYLIC ACID/1,4-/, 43 45 63 65 75 95; SEBACIC ACID, 43 45 63 65 75 95; METHANESULFONIC ACID, 43 45 63 65; METHANESULFONYL CHLORIDE, 43 45 63 65 75 95; HEXAMETHYLENEDIAMINE, N,N'-DIMETHYL-, 45 65; DODECANEDIAMINE/1,12-/, 45 65

**Figure 18.** IFI indexing for blends record U.S. 3637601.

examples are a mixture of propylene homopolymer and ethylene/propylene copolymer or a mixture of a polyamide and a polyester, where both polymers are made from aliphatic diacids. With the present indexing methods, it is very difficult to determine which diacid goes with which component of the mixture.

In the IFI Comprehensive Database, monomers can in general be structurally well-defined using compound terms or fragmentation codes. Their use in homopolymers or in copolymers can be defined with roles. The only linking in the IFI Databases is between structural fragments and between roles and the terms that they modify. Thus all polymers in a patent are combined in a single index field, whether they are present in the record as separate polymers or in mixtures or blends. For this reason, many false drops are retrieved in searching for blends in the Comprehensive Database.

For example, to search for blends of a polypropylene with nylon 66, the strategy should link adipic acid (50028) with roles (45, 55, 65) and hexamethylene diamine (50337) with roles 45, 55, and 65. These linked groups or the term polyhexamethylene adipamide (4213) linked with roles 10, 20, and 30 would be combined with the terms for propylene (50569) with roles 41, 51, and 61 or polypropylene (4267) linked with roles 10, 20, and 30. These groups would then be combined with the terms for a blend using "and" logic (Figure 17). In IFI's Indexing and Search Manual, it is indicated that polymers in mixtures should be searched using the roles that indicate the presence of the polymers unless their preparation or further use is described. However, to cover all possibilities, all the possible roles must be used.

IFI is very literal on indexing blends. If the patent says mixture, they will index mixtures (3417); if a blend, they will index blends (636). Other terms that could be used are alloys/polymers (8143), composites (8062), and composites as a "search only term, STO" (1208).

This strategy looks relatively straightforward, and it will provide the best recall. However, many false drops will result. For example, if a patent record which contained both a polypropylene blend and a polyamide of adipic acid also contained a different polyamide from a different diacid with hexamethylene diamine as one of its monomers, it would also be retrieved by this strategy and would be a false drop.

An example of such a false drop is shown in the abridged IFI reference shown in Figure 18. In this patent, hexamethylene diamine and terephthalic acid have formed the polyamide.

S1 AM=(050(S)688(S)141(S)160(S)206(S)207(S)040)

S2 S1 AND KS=(1723 AND 1450 AND (1283 OR 3174) AND 0248 AND (0218 OR 0219))

S3 S2 AND KS-3174

S4 S1 AND AM-(01& OR 01- OR 012 OR 010) OR S2 AND AM=011 OR S3

**Figure 19.** WPI strategy for blends search: polypropylene with nylon 66.

Patent Family: EP 315167 JP 1236208 US 4946918

Plasdoc Key Serials: 0013 0016 0020 0035 0037 0038 3002 0209 0210 0219 0044 0226 0239 0248 0304 0306 0307 3160 3161 0376 0377 0493 0500 3011 0535 0759 0787 0836 1096 1156 1275 1276 1277 1279 1282 1283 3174 1285 1291 3178 3179 1292 1294 1306 1319 1323 1355 1384 1450 1462 1511 1588 1592 1602 1606 1630 1634 1665 1669 1672 1676 1679 1683 1686 1690 3111 1723 1737 1804 3135 1990 1999 2002 2014 2021 2318 2334 2336 2378 2393 2394 2396 2465 2467 2507 2544 2545 2585 2632 2635 2667 0880 1417 1040 1033 1054 0279 1041 1418 1214 1235

**Figure 20.** WPI indexing for blends record EP 315167, Plasdoc Key Serials.

The examples that have been shown were blends of an addition polymer and a condensation polymer. If both components of the blend were condensation polymers, there would be another monomer to deal with, and the potential for cross indexing of polymer information would be increased, which would increase the number of false drops.

In Derwent's WPI Database, the structural nature of the monomer is not well defined unless it is one of a limited number of monomers with its own code. However, Derwent does link all components of a given polymer together, and each polymer has its own record. This should eliminate false drops due to multiple polymers in the same patent record. But this will not eliminate false drops that result from different polymers in a mixture or blend, since all the components of a blend are always in the same index record.

Derwent treats blends, alloys, and mixtures the same using the Plasdoc Code 040 for them, and the manual codes A07-A through A07-A04F are also used depending on the types of polymers that are blended. Composites are also indexed as blends except that their nonpolymeric components are indexed in the same record.

Using the same example as in the IFI section, the search strategy for polypropylene blends with nylon 66 is shown in Figure 19, where 050(S)688 are the codes for polypropylene homopolymer, 141 is for polyamides, and 160 is for adipic acid. The codes 206(S)207 are used for hexamethylene diamine, and 040 is the term for blends. The Key Serial Terms are 1723 for hexamethylene diamine, 1450 for adipic acid, 1283 for polyamides, and 3174 for nylon 66. The Key Serials are more precise, precoordinated terms that are used for indexing since 1978.

Because of all the information that is put on a single polymer record, there tends to be many false drops, but not as many as in the IFI system since Derwent will put different blends in separate polymer records. Examples of the type of false drops that will be retrieved are shown in the two abridged WPI records for the patent family EP 315167/JP 1236208/U.S. 4946918 in Figures 20 and 21. This patent describes blends of polypropylene and polyoxyalkylene derivatives, and blends of nylon 66 and polyoxyalkylene derivatives. All of the Key Serial Terms are shown in Figure 20. Figure 21 shows that the patent record contains all of the polymer fragment codes required for the search logic.

Patent Family: EP 315167 JP 1236208 US 4946918

Polymer Fragment Codes (AM): *101* 014 02& 028 034 039 040 041 046 047 05- 050 055 056 06- 061 062 063 064 066 067 071 072 074 075 076 077 080 081 082 09- 091 093 104 105 106 117 122 130 131 138 139 140 141 143 144 147 150 151 155 157 158 160 163 166 169 170 171 173 180 185 189 192 193 198 200 202 203 205 206 207 213 214 226 229 230 231 239 240 27& 27- 28& 31- 316 332 334 335 336 37- 38- 392 394 396 398 402 414 417 419 427 456 461 463 476 50& 531 55& 551 56& 567 570 573 575 58- 583 589 604 608 681 684 688 692 720 723 724 726

**Figure 21.** WPI indexing for blends record EP 315167, polymer fragment codes.

In Chemical Abstracts, "blends", "composites", and "alloys" are used as terms in the CA File to indicate the physical combining of two or more polymers in a homogeneous or heterogeneous system. Composites generally also contain a nonpolymeric material as well.

The CAS manual *Searching for Polymer Information in CAS Online* states that blends should be searched with either the appropriate controlled vocabulary headings (polymer classes) or CASRN (CAS Registry Numbers) for the component polymers linked with the terms blends, alloys, or composites. The term "mixture" is not indexed for these materials.

If each of the components of the mixture have their Registry Numbers together with the modifier terms of blends/alloys/composites on the same link, it should be possible to obtain very precise retrieval of these materials. In fact, the cases where the Registry Numbers of all the components are present in the same index field (i.e., linked) with the "blends" terms are artifacts of the online loading. If the records from an online search are compared with those from an ISS (CAS current awareness) search of the CAS master file, the ISS records will show two or more index fields while the CAS online file has one field. CAS combines index fields with the same modifying phrase in the online version. The record created appears to be accurately indexed, but in fact information is lost; i.e., it is not searchable. CASRN can only be searched linked to the modifier phrase terms; they can not be linked together. In our experience, the ideal retrieval situation (linkability of Registry Numbers) is not searchable in most cases. Generally, the Registry Number of one of the components of a blend is linked with the "blends" terms and names (common or trivial) for the other components. This indexing is then repeated for the other components of the mixture but separate index fields.

Of course, searching for components by name(s) is less precise and usually less comprehensive than searching by CASRN. In addition, use of compound description other than CASRN does not allow for comprehensive substructure searching.

One strategy to conceptually link the required groups would be to "and" the registry numbes together and then link them with other terms. If this is attempted, an error message from the Messenger System will result. The CASRN must be first linked (separately) with the compound names and "blends" terms, and then these groups must be "anded" together.

This method for finding information on polymer blends does work.

(1) Search the CASRN for each component. Alternatively, if appropriate, search the generic controlled vocabulary polymer class name (e.g., "polyamides").
(2) Search for the "blends" terms.
(3) Search for text modifier or common names for each component.
(4) Search each CASRN (or class name) linked to the "blends" terms.

File Registry

L1 25085-53-4 or 26063-22-9 or 9003-07-0
L2 25038-54-4 or 32131-17-2

File CA

L3 L1 [Polypropylene Registry Numbers]
L4 L2 [Nylon Registry Numbers]
L5 Blend# or Alloy# or Composite#
L6 L3 [Polypropylene Reg. Num's.] (L) L5 [Blends Terms]
L7 L4 [Nylon Reg. Num's.] (L) L5 [Blends Terms]
L8 L6 and L7
L9 Polypropylene or Polypropene
L10 Nylon(W)6 or Nylon(W)66 or Poly(W)hexamethylencadipamide or Polycaproamide or Polycaprolactam
L11 L6 (L) L10
L12 L7 (L) L9
L13 L9 (L) L5
L14 L10 (L) L5
L15 L13 and L14
L16 L8 or L11 or L12 or L15

**Figure 22.** CA strategy for blends search: polypropylene with nylon 6 or nylon 66.

TI Composites of ultrahigh-molecular-weight polymers and their manufacture

PI US 4944974

IT 9002-89-5, Poly(vinyl alcohol) 9003-07-0 , Polypropylene 25014-41-9, Polyacrylonitrile 25038-54-4 , Nylon 6, properties 25038-59-9, Poly(ethylene terephthalate), uses and miscellaneous 25085-53-4 , Isotactic polypropylene 26161-42-2 33135-50-1, Poly(L-lactide)
(ultrahigh-mol. wt., composites from sheets and wovens, with high modulus and strength)

**Figure 23.** CA indexing for blends record U.S. 4944974.

TI Preparation of olefin graft polymers for use in polymer blends

PI DE 3909273

IT 9003-07-0 9071-17-4 24937-78-8D, hydrolyzed 24979-70-2, Poly(p-vinylphenol) 25497-66-9 79331-75-2 108548-63-6, Laurylactam-polytetramethylene glycol block copolymer
(blends with nylon 6, compatibilizing agents for, graft polymers as)

IT 25038-54-4 , Poly[imino(1-oxo-1,6-hexanediyl)], uses and miscellaneous
(blends with plastics, compatibilizing agents for, graft polymers as)

**Figure 24.** CA indexing for blends record DE 3909273.

(5) These latter sets (4) are then "anded" together.
(6) Each CASRN/blends set (4) is then linked to text modifier name sets for each of the other components.
(7) Text modifier names for each component are then linked to "blends".
(8) All of these sets (7) are "anded" together.
(9) Finally, sets (5), (6), (7), and (8) are combined ("ored") for the final result.

This is best illustrated with blends of polypropylene and nylon 6 or nylon 66. The Registry Numbers for polypropylene are 26063-22-9 for syndiotactic polypropylene, 25085-53-4 for isotactic polypropylene, and 9003-07-0 for "ordinary" polypropylene. The Registry Number for nylon 6 is 25038-54-4 and 32131-17-2 for nylon 66. The text modifier terms for polypropylene are polypropylene and polypropene. The text modifiers for the nylons are nylon 6, nylon 66, poly(hexamethyleneadipamide), polycaproamide, or polycaprolactam. There are other names that could be used as well, and this is another reason that condensation polymers are hard to search. There are usually many possible synomyns. The blend terms are blend#, alloy#, and composite#.

The search strategy is shown in Figure 22. If a strategy like this is not used, good references will be missed but many false drops are possible because of records that describe more than one type of blend. For example, in searching for blends of polypropylene and nylon 6 or nylon 66, one obtains refer-

TI Polyoxyalkylene derivative-based copolymer compatibilizers for synthetic polymer blends

PI EP 315167

IT 25038-54-4, Nylon 6, uses and miscellaneous
(synthetic polymer blends, Amilan CM1017, compatibilizers for, polyoxyalkylene deriv.-based copolymers as)

IT 32131-17-2 , Nylon 66, uses and miscellaneous
(synthetic polymer blends, Leona 1300 S, compatibilizers for, polyoxyalkylene deriv.-based copolymers as)

IT Polypropylene 9003-08-1, . . . .
(synthetic polymer blends, compatibilizers for, polyoxyalkylene deriv.-based copolymers as)

**Figure 25**. CA indexing for blends record EP 315167.

TI Fiber-reinforced polyamide-thermoplastic blends

PI DE 3840374

IT 9003-07-0 24936-68-3, uses and miscellaneous 25037-45-0 25212-74-2, Poly(thio-1,4-phenylene) 61128-24-3 61128-46-9
(blends with polyamides, fiber-reinforced, melt flow improvers and couplers for)

IT 25038-54-4, Poly[imino(1-oxo-1,6-hexanediyl)], uses and miscellaneous
(blends with thermoplastics, fiber-reinforced, melt inflow improvers and couplers for)

**Figure 26**. CA indexing for blends record DE 3840374.

ences like U.S. 4944974 (Figure 23). The Registry Numbers for isotactic polypropylene and nylon 6 plus "composites" are in the same index field. In DE 3909273 (Figure 24), the registry number for polypropylene is linked to blends and to the term nylon 6 in one index field. Both patents appear to be relevant. However, EP 315167 is also retrieved (Figure 25). Here, one index field contains the Registry Number for nylon 6 linked to blends linked to polyoxyalkylenes. The next index field contains the registry number for nylon 66 linked to blends linked to polyoxyalkylenes. A third field contains the Registry Number for polypropylene linked to polyoxyalkylenes. This is not the subject of the search.

Additional generic terms or polymer classes may also be indexed. For example in DE 3840374 (Figure 26), one index field (IT) contains the CASRN for polypropylene linked to polyamide blends, and another IT field contains the CASRN for nylon 6 linked to thermoplastic linked to blends. This reference may very well be a key reference, but one cannot be sure from the indexing. Since there may be more than one polyamide blend, it is not obvious if the blend involving nylon 6 is also a blend with polypropylene.

This record was retrieved from presumably the most precise part of the search: the "and" combination of the CASRN/blends sets for each of the two components. However, the rest of the record or the original document must often be examined to determine if the retrieval is by coincidence or if both description of blends are indeed describing the same blend. Use of more generic terms (i.e., common names) enhances search recall but also decreases precision (i.e., more false drops). In this example, the use of "propylene" instead of the polypropylene CASRN also retrieves blends of modified or derivatized polypropylene, which may or may not be of interest. Use of "polyamide" or "polyolefin" (or "alkenes, polymers") blends may retrieve some good hits (especially in older portions of the file), but usually the specific components are not those of interest.

## STEREOCHEMISTRY

Stereoregularity usually is encountered with addition polymers. Stereochemistry in addition polymers is not necessarily dependent on asymmetric monomers but is observed in vinyl polymers with asymmetric centers that appear only after polymerization. For example, propylene can be polymerized to stereoregular polypropylene. For this type of stereoregular addition polymer, the whole polymer is described as isotactic (all groups in one plane) or syndiotactic (groups alternate between planes).

With the exception of polyalkylene oxides, polyalkylene amines, polylactones, or polylactams, stereoregular condensation polymers usually occur only in polymers of asymmetric monomers (e.g., polypeptides). These polymers are usually described in terms of their monomers using the R and S designations.

Chemical Abstracts, Derwent, and IFI handle the indexing of stereoregularity differently. In CA each stereoregular polymer has its own registry number. For polymers where the stereoregularity varies by blocks, the polymers are registered as the non-stereoregular (atactic) polymers. The stereochemistry of the different blocks is included in the CA File as text modifiers.

In the Derwent files, there is one very generic index term, stereoregular polymers (586), which covers all forms of stereochemistry. There is also a term for atactic or amorphous polymers (029).

In the IFI indexing there are several stereochemical terms that can be used for retrieval, atactic (440), isotactic (2980), syndiotactic (5425), and stereospecific (5295).

## CONCLUSION

In conclusion, for a number of reasons, searching condensation polymers is inherently more difficult than searching addition polymers. Comprehensive retrieval is often accomplished only with a large loss in precision. More precise indexing by all of the abstracting and indexing organizations would greatly assist the quality of retrieval. Linking of appropriate monomers with both polymer type and aggregation type is a necessary but possibly insufficient condition. For example, blends should be indexed as their component polymers (either specifically or as SRU's), both linked together and linked to the blend concept. In cases where the individual components of a polymer are known, these components should be linked together in a manner that will keep them separate from the components of any other polymer in the blend. Structural information should be indexed by a substructure system (CAS Registry System or Markush DARC) or by fragmentation. None of the services mentioned indexes at this level at this time, although Chemical Abstracts comes the closest. However, their subject and country coverage is not complete enough for many who search for chemical patent information.

## REFERENCES AND NOTES

(1) Buntrock, R. E. Documentation and Indexing of C4 Compounds: Pathways and Pitfalls. *J. Chem. Inf. Comput. Sci.* **1991**, *29*, 72–78.
(2) See other papers from this symposium published in this issue.