The monomers in appropriate polymer roles are indexed as well as the polymer class terms and the specific copolymer term ACRYLONITRILE-BUTADIENE COPOLYMER.

Obviously, this procedure allows great flexibility in specificity level when searching. A patent so indexed would be selectively retrieved in a search for the specific copolymer. It would also be easily retrieved in a search for any butadiene or any acrylonitrile polymer or even more broadly any nitrile or any conjugated polyene polymer.

Polymers not included in the seven classes just described are handled somewhat differently. For convenience, these are called Other Polymers. They include (1) polymers containing a repeating backbone structure which is not one of the common types, and (2) polymers having no consistent repeating unit, e.g., polyimides, organometallic polymers. An analogous set of roles is used for these polymers.

The polymer monomers may be described either by the IFI Compound Term vocabulary or by the IFI fragmentation system. Each compound in the Compound Term vocabulary is also described via this fragmentation system so that in a search for polymers prepared from unsaturated isocyanates the requester is able to combine the IFI fragmentation system with the polymer role system for effective retrieval of pertinent information.[4]

CONCLUSION

We believe the polymer indexing–retrieval system we have just described is a viable approach to overcoming some of the obstacles inherent in handling polymer patents: the variety of options for identification, the variety of user requirements and interests, the volume, and the cost relationships. By using combinations of specific polymer names, prescribed starting monomers, roles, and polymer class terms, the searcher is able to handle questions ranging from the very specific to the generic. The system is able to manipulate a large volume of material and is designed to be cost effective from an indexing cost versus search cost point of view. Using this system we feel we are able to make polymers and patents mix more easily.

LITERATURE CITED

(1) J. Maynard, "Understanding Chemical Patents", American Chemical Society Publication, Washington, D.C., 1978, p 23.
(2) L. E. Rasmussen and J. G. van Oot, "Operation of DuPont's Central Patent Index", *J. Chem. Doc.*, **9**, 201–206 (1969).
(3) J. L. Schultz, "Polymer Nomenclature, Classification and Retrieval in the DuPont Central Report Index", *J. Chem. Inf. Comput. Sci.*, **15**, 94–100 (1975).
(4) M. Z. Balent and J. M. Emberger, "A Unique Fragmentation System for Indexing Patent Literature", *J. Chem. Inf. Comput. Sci.*, **15**, 100–104 (1975).

Fossil Fuels in *Chemical Abstracts*†

CHARLES W. MOULTON
Chemical Abstracts Service, Columbus, Ohio 43210

Received December 28, 1978

Chemical Abstracts Service provides a broad array of information and services for those who have an interest in fossil fuels. These services range from the time-honored CA Abstract Issues themselves, with their several types of indexes, through subsets of the printed abstracts selected and packaged according to various topical interests, to computer-readable tape files compiled for different, but complementary purposes.

Information on fossil fuels has been abstracted and indexed in *Chemical Abstracts* (CA) since its inception 70 years ago. The very first issue, January 1, 1907, carried 18 abstracts in a section entitled "Fuel, Gas, Coke", and 11 more were included in what was then an entirely separate section devoted to the patent literature. And in a section entitled "Petroleum, Asphalt, Wood Products", the only paper abstracted dealt with pitch and terpenes of pine and fir; the single pertinent patent was concerned with the refining of hydrocarbon oils.

In contrast, Issue 2 of Volume 89, dated July 1978, contained nearly 350 abstracts in the present Section 51, "Fossil Fuels, Derivatives, and Related Products". These numbers reflect not only the greatly increased interest in this field, but also the historic growth rate of the technical literature of some 8 to 9% per year.

THE ABSTRACTS

Chemical Abstracts Service (CAS) is charged with the responsibility of abstracting and indexing the chemical literature faithfully, as it is published, without exercising any critical evaluation as to its validity and/or intrinsic merit. Critical judgment is the responsibility of those who use CA. As distinct from certain other information services, CAS does not provide archival compilations of data; rather, it directs the user, through the abstracts and indexes (both for current work and retrospectively through the Collective Indexes), to the research papers, patents, conference proceedings, and books that report and discuss the scientific work carried out in the laboratories of the world. CA provides the access; others do the compiling.

Section 51 of the Abstract Issues of CA, "Fossil Fuels, Derivatives, and Related Products", is the principal section that deals with fossil fuels. The technical literature abstracted in this section encompasses the following aspects:[1]

(a) geochemistry: the origin, location, and description of deposits of petroleum, natural gas, oil shales, tar sands, coal, and peat;
(b) the chemistry and chemical engineering of extraction, production, processing, and usage;
(c) products and derivatives: synthetic fuel gases, gasoline, jet and diesel fuels, naphthas, lubricants and greases, bitumens and asphalt, coke, etc.;
(d) analysis of fossil fuels and their derivatives;
(e) organic compounds produced from carbon monoxide and hydrogen;
(f) synthetic lubricants and hydraulic fluids.

Explicitly excluded from this section are studies concerned primarily with the treatment of automotive exhausts and stack

† Presented, in part, before the Division of Chemical Information, Symposium on "Fossil Fuels Information Systems and Services", 174th National Meeting of the American Chemical Society, Chicago, Ill., Aug 31, 1977.

0095-2338/79/1619-0083$01.00/0 © 1979 American Chemical Society

0. Reviews

Petroleum, Derivatives, and Related Products

1. General and geochemistry
2. Production
3. Preconversion, processing
4. Natural gas
5. Manufacture of gasoline hydrocarbons (including catalysts)
   - Alkylation
   - Conversion
   - Cracking
   - Hydroforming
   - Hydrogenation
   - Isomerization
   - Polymerization
   - Reforming (Platforming)
   - Separation (molecular sieves)
6. Gasoline formulations
   - Analysis
   - Additives and gum inhibitors
   - Blends
   - Octane number improvement and determination
7. Lubricating oils
   - Analysis
   - Solvent refining
   - Dewaxing
   - Compounding and blending
   - Additives (pour-point depressants, gum and corrosion inhibitors)
   - Cutting oils
   - Slushing compounds
   - Spindle oil
   - Transformer oil
   - Greases
8. Synthetic lubricants
9. Other fractions
   - LPG and other gases
   - Diesel fuel
   - Gas oil
   - Kerosine
   - Light oil
   - Naphtha
   - Spirits (mineral)
10. Residues
    - Asphalts and emulsions
    - Bitumens
    - Coke
11. Special products
    - Acid-sludge recovery
    - Naphthenic acids
    - Petroleum resins
    - Sulfonates
    - Waxes
    - White oils
    - Antifreeze compositions
12. Combustion
13. Chemical engineering
    - Equipment design
    - Corrosion problems
    - Lubrication technology
14. Shale processing
15. Tar-sand processing

Figure 1. Petroleum subsection arrangement.

Coal and Coal Derivatives

16. General studies
17. Classification
18. Analysis and composition
19. Chemical properties
20. Physical properties
    - Color
    - Texture, fracture, hardness, and friability
    - Specific gravity
    - Thermal properties
    - Electrical properties
    - Optical properties including infrared, ultraviolet, X-ray, and reflectivity
21. Preparation
22. Storage
23. Briquetting
24. Combustion (excluding physicochemical studies on gases)
25. Carbonization and its products
    - Coke
    - By-products
    - Tar
    - Gas
    - Waste liquor
26. Gasification
27. Gas purification
28. Hydrogenation
29. Conversion
    - Synthetic gaseous and liquid fuels
    - Chemicals
30. Mine gases
31. Lignite, peat, and brown coal

Figure 2. Coal subsection arrangement.

gases, paving compositions, and nonchemical aspects of plant engineering, mining, and petrography.

The subject matter of this section is arranged systematically into two major subdivisions, "Petroleum, Derivatives, and Related Products" and "Coal and Coal Derivatives". As for all CA sections, abstracts of those papers that are classified as reviews (including bibliographies, lectures, and other types of publications that contain no new information) appear together ahead of all others in a subsection that is numbered 0. All other papers are arranged into 31 subsections, 15 in the "petroleum" subdivision (Figure 1) and 16 in the "coal" subdivision (Figure 2). Abstracts that deal with the patent literature are grouped at the end of the section, following the nonpatent literature, with the same subject arrangement. As is common practice throughout CA, announcements of the titles of books concerned with the subject (including book-length bibliographies and separately published conference proceedings) appear as a single grouping immediately ahead of abstracts on the patent literature.

Placement in a particular subsection is governed by the emphasis of the original document. Subjects pertaining to more than one of the subsections are commonly discussed in a single document, so that the stated or implied intent of the author(s) is taken into account for the purpose of subsection assignment. As any given document is abstracted only once in CA, arbitrary assignment must be made when there is essentially equal stress on topics appropriate to more than one of the subsections.

As is so frequently the case for the many topics covered by CA, papers dealing with certain aspects of fossil fuels can be assigned to any number of other sections, depending upon the principal emphases. For example, certain information related to geological sources is to be found in the section entitled "Mineralogical and Geological Chemistry" (Section 53), while engineering processes of related interest will appear in the engineering sections that deal with apparatus, plant equipment, and unit operations and processes (Sections 47 and 48).

Industrial wastewaters and mine drainages are dealt with in "Sewage and Wastes" (60), and pollution is treated in the biochemical section "Toxicology" (4) and in the applied sections "Water" (61) and "Air Pollution and Industrial Hygiene" (59). Reactions of interest for refining and conversion can appear in the synthetic-organic sections (23–24) or in that section that deals with catalysis and reaction kinetics (67).

For those abstracts of papers, patents, etc., that deal with fossil fuels, but are placed in sections other than 51, cross references appear at the end of Section 51 under the two headings: "For papers of related interest see also Section:" and "For patents of related interest see also Section:". In addition to the section numbers, these cross references carry CA abstract numbers and titles to the papers, patents, etc.

THE INDEXES

Since the usefulness of a secondary publication depends to such a great extent on the adequacy of its indexing, the content of CA is indexed and cross-indexed in a variety of ways.

The Keyword Index printed in each of the Abstract Issues serves a current-awareness purpose, directing the searcher to those abstracts that deal with a particular subject throughout that particular issue of CA. An example of entries in this index is shown in Figure 3. This is an alphabetically arranged, permuted keyword-in-context (KWIC) index, characterized by an uncontrolled vocabulary and an essentially unarticulated word string of restricted length, seldom more than four or five words. It is based for the most part on the abstracts alone, and so is not an "in-depth" index to the entire content of the documents abstracted.

The Subject Indexes, associated with each of the semiannual volumes of CA (and compiled into the ten-volume Collective Indexes issued every five years), are, on the other hand, controlled vocabulary indexes insofar as the subject *headings* (and certain subordinate material) are concerned. Since they are compiled as a result of more detailed analyses of the documents abstracted, they provide considerably greater depth of indexing.

Figure 4 illustrates some of the subject headings that are concerned with fuel gases. Such headings as "Fuel gases", "Natural gas", and "Natural gas condensates" refer to these particular subjects in a general way, rather than to the specific chemical compounds involved. Substance class headings of

Native
platinum analysis ruthenium isotope 156852c
Natrolite
ion exchange potassium 149546c
Natural
gas absorption sweetening review 148947x
gas analysis noble gas 156820r
gas analysis titrator 149019h
gas combustion gas stove 151682n
gas combustion toxic component 151764r
gas drying purifn 149027j
gas enthalpy 153675m
gas equil liq 149023e
gas geochem isotope effect 149010y 149012a
product drug review 152590t
rubber abrasion model 147923z
rubber blend hardness 147893q
water biophilic compd reaction 152336q
water tritium USSR 152207y
Naval
oil detn water detergent 152514w
Nebula
diffuse spectra shadow 155370g
emission Large Magellanic Cloud 155320r

Figure 3. Keyword Index.

Natural gas	Natural gas prospecting
Natural gas condensates	
Fuel gases	Fuel gas manufacturing
Methane - Propane - Hydrogen - Carbon monoxide - etc.	

Figure 4. Fuel-Gas Index headings.

Petroleum	Petroleum prospecting
Petroleum wells	Petroleum recovery
Oil shale	Shale oil
Oil sand	
Kerogen	Bitumens
Petroleum refining	Petroleum refining catalysts
Petroleum refining residues	Petroleum products
Gasoline - Kerosine - Naphtha - Fuel oil - Fuels, diesel - Fuels, jet aircraft - etc.	

Figure 5. Petroleum-related index headings.

this type and headings that refer to processes (e.g., "Fuel gas manufacturing") and to scientific concepts (e.g., "Heat of combustion") are grouped into the section of the Subject Indexes that is designated the General Subject Index.

Also included in Figure 4 are several of the substance headings for specific compounds that find use as gaseous fuels. These headings appear in that part of the Subject Index devoted to elements and compounds, designated the Chemical Substance Index. The Chemical Substance Index also carries for each specific substance its related Registry Number. This is a uniquely assigned number for each substance, related only to composition and structure, independent of how it may be named. Thus all synonyms for a particular substance are interconnected through its Registry Number.

Some of the index headings that are related to petroleum and to coal are given in Figures 5 and 6, respectively.

Indexing policies are documented in the Index Guide, an adjunct publication to the Subject Indexes. The policies are stated in the form of extensive general introductory descriptive material together with scope notes and cross references appropriate to particular headings. An example from the Index Guide of scope notes and cross references appearing under "Coal" and "Coal, brown", is shown in Figure 7.

In addition to the Keyword and Subject Indexes, there are the following:

(a) Author Indexes—for access to the abstracts by means of an alphabetical listing of document authors, inventors, and assignees of patented material, corporations, governmental agencies, etc.;

(b) Formula Indexes—for access by means of molecular formulas, arranged alphabetically by element symbol, except that the symbol for carbon always appears first when present, and is then followed immediately by that for hydrogen; formulas are provided both for compounds that are cited in the abstracts and also for those that are selected from the documents for inclusion in the indexes;

(c) Index of Ring Systems—to provide the basic parent names for ring structure skeletons, arranged by number, size, and elemental constitution of the rings, thereby giving access to abstract references under the names in the Chemical Substance Index of the compounds that contain those constituent ring systems;

(d) Numerical Patent Indexes—for access to abstracts on the chemical patent literature by means of patent numbers, arranged sequentially under the names of the issuing countries;

(e) Patent Concordance—for access to the patent abstracts for equivalent patent specifications issued by other countries, arranged by country and number, with references to the abstracted patents and the CA abstract numbers for the first citations.

Of these, an Author Index, a Numerical Patent Index, and a Patent Concordance are included in each of the abstract issues. These are then compiled into both the Semiannual Volume and the Five-Year Collective Indexes. The Formula Index and the Index of Ring Systems are issued with the Volume Indexes and are also compiled for the Collective Indexes.

Coal	Coal, brown
Peat	
Clarite - Durain - Vitrinite - etc.	
Mining	Mines
Carbonization and Coking	Coke
Fuel gas manufacturing	

Figure 6. Coal-related index headings.

Coal
Anthracite and bituminous coals are indexed at this heading. Brown coal and lignite are indexed at *Coal, brown*. Specific lithotypes, microlithotypes and macerals are indexed at such headings as *Clarite, Durain, Vitrinite*. Products derived from coal are indexed at such headings as *Coke, Fuel gases, Tar*
briquets from —— see *Fuel briquets*
carbonization or coking of —— see *Carbonization and Coking*
firing with
see
Burners
Firing of furnaces
Furnaces
gasification of —— see *Fuel gas manufacturing, gasification*
mines for —— see *Mines*
mining of
see
Explosives
Mining
smoke from —— see *Smoke*
stokers or feeders for —— see *Feeding apparatus*
Coal, brown
Lignite is also indexed at this heading. Specific lithotypes, microlithotypes and macerals are indexed at such headings as *Clarite, Durain, Vitrinite*. Products derived from brown coal or lignite are indexed at such headings as *Coke, Fuel gases, Tar*
briquets from —— see *Fuel briquets*
carbonization or coking of —— see *Carbonization and Coking*
gasification of —— see *Fuel gas manufacturing, gasification*
mines for —— see *Mines*
mining of —— see *Mining*
smoke from —— see *Smoke*
wax of
see
Montan wax
Waxes and Waxy substances
brown-coal
xylite —— see *Xylite (lignitous)*

Figure 7. Example from Index Guide.

SPECIALIZED SERVICES

The heart of the CAS services remains *Chemical Abstracts* itself, the printed Abstract Issues with their attendant indexes. But in addition, there is a wide array of services made available in various formats for specialized purposes.[2] Several of these pertain to the field of fossil fuels.

Among the services available in print, the Section Groupings provide the total content of the Abstract Issues in five packages: the biochemical, organic, macromolecular, applied and engineering, and physical and analytical groupings. Section 51 as a whole is included in the grouping that is designated "CA Applied Chemistry and Chemical Engineering Sections". Complete bibliographic information is included, as well as the Keyword Index entries for the entire issue of CA from which the particular grouping is extracted.

"Coal Science and Process Chemistry" is representative of one of the newest family of services, *CA Selects*. This is a printed current-awareness service, issued biweekly, which includes the bibliographic information and abstracts that appear throughout CA dealing with coal—its liquefaction, gasification, carbonization, properties, analysis, composition and combustion—mine gases, and brown coal. Thus all abstracts that have anything to do with coal, in whatever section they appear, are collected into a conveniently scanned publication. This publication, along with more than 70 others in various specialized subject areas, was recently introduced to provide an inexpensive current-awareness alternative to the many such computer-readable services. The information provided by the various *CA Selects* topics is extracted from the CAS database by computerized retrieval that is based on custom-designed search profiles.

CA Condensates (CACon) and *CA Subject Index Alert* (CASIA) are computer-readable tape services, issued biweekly. The former is a compilation of the bibliographic information, section numbers, and keywords from the Abstract Issues; abstracts are not included. CASIA provides the index entries that are subsequently published in the semiannual Subject and Formula Indexes; these index entries are associated with the corresponding abstracts in the printed issues through the abstract numbers. Section and subsection numbers and Registry Numbers for specific substances are included in CASIA.

Lastly there is the tape file *Energy*, which includes abstracts, bibliographic information, section and subsection numbers, keywords, and index entries for a selected group of energy-related CA sections. Section 51 appears in this file as a whole. The other sections included are those that deal with propellants and explosives (50); with electrochemistry (72) and with electrochemical, radiational, and thermal energy technology (52); with thermochemistry and thermal properties (69); and with nuclear phenomena and technology (70 and 71).

REFERENCES AND NOTES

(1) "Subject Coverage and Arrangement of Abstracts by Sections in *Chemical Abstracts*," 1975 edition, Chemical Abstracts Service, Columbus, Ohio.
(2) The CAS database concept is described by R. E. O'Dette, *J. Chem. Inf. Comput. Sci.*, **15**, 165–9 (1975).

A Problem-Oriented Analysis of Database Models

NADIA THALMANN*†
Section Systèmes d'Information, Faculté des Sciences de l'Administration, Université Laval, Québec, Canada

DANIEL THALMANN
Département d'Informatique et de Recherche Opérationnelle, Université de Montréal, Montréal, Canada

Received January 17, 1978

Which is the most convenient database model considering specific applications? The goal of this paper is to try to answer this question by the use of a chemical example. Examples of requests describe the problems of insertion, deletion, and updating; these requests are analyzed for the hierarchical model and are expressed in a relational language defined by the authors and in Socrate for the network model.

1. INTRODUCTION

An increasingly important aspect of commercial data-processing activities is database management systems (DBMS). First, two questions have to be answered: what is a database and why are DBMS necessary?

Engles[9] defines a database as a collection of stored operational data used by the application systems of some particular enterprise. We may accept this definition if the word "enterprise" means an organization such as a bank, a school, or a hospital. A DBMS is necessary for the following reasons: (i) the operations of a file system will refer to entities in the physical part of the database description, (ii) logical errors have to be checked, (iii) protection against misuse has to be assured, and (iv) standardization should be assured.

The DBMS world often seems very confusing because of the variety of options available to implement such systems. However, most authors[2,7,15] consider three general database models: (i) the hierarchical model, (ii) the network model, and (iii) the relational model.

Two other models have been proposed: the entity set model by Senko[12] and the entity-relationship model by Chen.[3] We shall not discuss these two models in this paper as their qualities are similar to those of the relational model.

If some authors[2,7] have discussed the advantages and disadvantages of each model, a major tendency in database management literature and systems is to choose always examples of employees, ages, departments, and so on. It is not surprising because DBMS were first designed for management applications, but today, databases take an important place in all science areas.

†This work is partly supported by the Swiss National Fund for Scientific Research, while on leave of absence from the Department of Chemistry of the University of Geneva, Switzerland.

0095-2338/79/1619-0086$01.00/0 © 1979 American Chemical Society