Separation Science and Technology
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713708471

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To cite this Article Dowell, W. J. Mc , Roddy, J. W. and Michelson, D. C.(1981) 'A Data Base for Separations Chemistry', Separation Science and Technology, 16: 9, 1291 — 1298
To link to this Article: DOI: 10.1080/01496398108057611
URL: http://dx.doi.org/10.1080/01496398108057611

SEPARATION SCIENCE AND TECHNOLOGY, 16(9), pp. 1291-1298, 1981

A Data Base for Separations Chemistry

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ABSTRACT

Computer retrieval of information related to hydrometallurgical separations from most data bases is limited and is also complicated because the terms *solvent extraction, ion exchange, chromatography,* etc. have widespread use in a variety of disciplines and widely varying meanings in each. A data base called *Separations Science Data Base*, designed specifically for retrieval of information needed in chemical separations problems, has been assembled. The indexing is structured in such a way as to allow accommodation of a variety of separations methods (distillation, precipitation, flotation, etc.), but liquid-liquid (*solvent*) extraction and solid-liquid ion exchange are being emphasized initially. The reference material can be retrieved not only in terms of the standard author, title, source, and date-of-publication entries, but also in terms of the substance separated (both those recovered and those rejected), the separations system and the separation agent used, the matrix from which the separation is effected, and the type of information in the reference.

BACKGROUND

The problem of effectively retrieving from the literature information on how to perform a specific chemical separation under specific conditions has become increasingly difficult in recent years. Of course, difficulties in information retrieval

exist for any subject area because of the rapid increase in the volume of technical literature over the past 20 years, although for many subjects the use of computer-searchable data bases has alleviated the problem to a large degree. However, such data bases have been less effective in the area of separations chemistry because this field cuts across the traditionally established scientific disciplines, and the key words or key terms used in separations chemistry have different meanings in these various disciplines. For example, the term *solvent extraction* indicates widely different things in biology, petroleum chemistry, and hydrometallurgy. Similarly, the term *ion exchange* is used to refer to liquid, resinous, and zeolite separations. These multiple meanings and inconsistencies in key word usage result in the separations chemist obtaining an unacceptably large percentage of unwanted material when searching existing data bases.

In addition to the above-mentioned problem, many important separations references are poorly indexed. A large body of information in solvent extraction and ion exchange separations related to hydrometallurgy and analytical chemistry was generated in government research programs in the mid 1940s to mid 1960s. Much of this information was originally classified secret, had limited indexing of any sort, and is not included in any computer-searchable data base. This lack of availability to the public has already resulted in some duplication of research effort.

To make all of the pertinent literature including the above-mentioned early reports more effectively and more readily available to the separations scientist, a data base designed specifically for the computerized storage and retrieval of information needed for the solution of chemical separations problems is being compiled. Initial entries are concerned primarily with solvent extraction, ion exchange, and related subjects, but a field called SEPARATION SYSTEM allows the inclusion and indexing of almost any type of separation; for example, distillation, flotation, or osmosis. The data base is stored on the ORNL computer system and is currently available in an on-line interactive mode through *DOE/RECON* (Department of Energy Remote Console) system.[1]

DISCUSSION

The searchable information fields are:

AUTHOR	SEPARATION SYSTEM
TITLE	SEPARATED SUBTANCE
DATE	SEPARATION AGENT
ABSTRACT	MATRIX
LITERATURE TYPE	TYPE OF INFORMATION

The fields in the left-hand column contain standard bibliographic information. Those in the right-hand column contain descriptor terms that are usually consolidated under one heading but are separated here into five categories. Carefully selected descriptor terms within these fields describe the information contained in a report or paper that is within that information classification. Dividing the index terms into these information areas makes the data base

```
ENTER:expand cobalt
>PROCESSING<
  EXPAND   IT=COBALT
    REF  DESCRIPTOR                  CIT  RT
    E01  IT=CHROMIUM -----------      8
    E02  IT=CHROMIUM(II)- ------      1
    E03  IT=CHROMIUM(III) -------    15
    E04  IT=CHROMIUM(III)- ------    10
    E05  IT=CHROMIUM(VI) -------     13
   -E06  IT=COBALT ---------------   102
    E07  IT=COBALT -------------     22
    E08  IT=COBALT ,- ------------    9
    E09  IT=COBALT(II) -----------   62
    E10  IT=COBALT(II)- ----------    4
    E11  IT=COBALT(II),- ---------    1
    E12  IT=COBALT(III) ----------    8
    E13  IT=COPPER ---------------  165
    E14  IT=COPPER +- ------------    1
    E15  IT=COPPER -- ------------   26
    E16  IT=COPPER ,- ------------    6
    E17  IT=COPPER(I) ------------    6
    E18  IT=COPPER(I)- -----------    1
    E19  IT=COPPER(II) -----------   55
    E20  IT=COPPER(II)- ----------    3
                                    -MORE-
ENTER:
```

Figure 1. The portion of SEPARATED SUBSTANCE index displayed as a result of command, "expand cobalt."

especially useful to the separations scientist since, by the use of appropriate combinations of terms from selected fields, information on specific separations under specific conditions can be retrieved.

This type of search is facilitated by two other features of the data base. First, since the primary purpose of most searches will be to retrieve information on the separation of various substances, the SEPARATED SUBSTANCE index has been made the default index on the RECON system; that is, a search for information on a separated substance can begin without specifying the SEPARATED SUBSTANCE index. Thus, the most useful kind of search is begun more easily. Each of the terms used in a field or category is listed in an alphabetical index, and portions of this index may be examined by an "expand" command. Thus, the command EXPAND COBALT will display to the user an index like that shown in Fig. 1. Second, the SEPARATED SUBSTANCE index contains notations giving additional information about the separation. For example, use of the name of the substance only indicates that the substance is extracted (or retained on column or

```
ENTER:expand ma=aqueous
>PROCESSING<
  EXPAND   MA=AQUEOUS
    REF DESCRIPTOR                CIT  RT
    E01 MA=ACETATE                 73
    E02 MA=ACID                  1374
    E03 MA=AIR                      9
    E04 MA=ALCOHOL                 18
    E05 MA=AMMONIACAL              79
   -E06 MA=AQUEOUS                904
    E07 MA=BASE                    99
    E08 MA=BIOLOGICAL
            MEDIUM                  2
    E09 MA=BORATE                  12
    E10 MA=BRINE                   23
    E11 MA=BROMIDE                 76
    E12 MA=CARBONATE               54
    E13 MA=CHLORIDE               794
    E14 MA=CITRATE                 30
    E15 MA=COMPLEXANT             211
    E16 MA=CYANIDE                  9
    E17 MA=FLUORIDE                77
    E18 MA=FORMATE                  4
    E19 MA=GAS                     30
                                  -MORE-
ENTER:
```

Figure 2. The portion of MATRIX index displayed as a result of the command "expand ma = aqueous."

filter) or that specific information on a separation was not given; the name followed by a space and a minus sign (−) indicates that the substance is rejected (not extracted or retained). Substances that can be optionally collected or rejected are followed by a space, a comma, and a minus sign (,−). Roman numerals indicate oxidation states and are given when known. The use of the indexes presented in this form allows the searcher to include or exclude as much of the material as is wished. For example, in Fig. 1 the searcher might want to see all references concerning cobalt separation, in which case E6 through E12 would be selected. To see references in which cobalt is rejected, E7, E8, E10, and E11 would be selected, and so on.

The next step in selecting reference material for a specific separation would be to choose a matrix from which the separation is to be made. Again the RECON EXPAND command allows the searcher to view the choices that are indexed, an example of which may be seen in Fig. 2. After selecting a matrix, combining the two sets with AND logic (combine 1 AND 2 or 1*2) produces a set of references in

```
ENTER:select copper
>PROCESSING<
   1      165  IT=COPPER
ENTER:select iron -
>PROCESSING<
   2       36  IT=IRON -
ENTER:select ma=sulfate
>PROCESSING<
   3      385  MA=SULFATE
ENTER:combine 1and2and3
>PROCESSING<
   4        4  1AND2AND3
ENTER:display 4/4/all
>PROCESSING<
DIS  4/4/000001-000004//1

<ACCESSION NO.> 00*0001602      *******1
<AUTHOR> Grinstead, R.R.
<TITLE> Copper-Selective Ion Exchange Resin with Improved Rejection: TMS
          Reprint No. 1
<SOURCE> 108th Annual AIME Meeting, New Orleans, Feb. 18-22, 1979;
          CONF
<DATE> Feb 1979

<ACCESSION NO.> 00*0000250      *******2
<AUTHOR> Vasilenko, L.F.; Nomodruk, A.A.; Soloshenkin, P.M.
<TITLE> 2-Mercaptobenzothiazole as a Selective Reagent for Extraction of
          Copper
<SOURCE> Izv. Akad. Nauk. Tadzh. SSR, Otd. Fiz.-Mat. Geol.-Khim. Nauk
          1975(4), 117
<DATE> 1975

<ACCESSION NO.> 00*0000237      *******3
<AUTHOR> Spivakov, B.Ya.; Lebedev, V.I.; Shkinev, V.M.; Krivenkova, N.P.;
          Plotnikova, T.S.; Kharlamov, I.P.; Zolotov, Yu.A.
<TITLE> Extraction of Elements with Trioctylamine from Iodide Solutions
<SOURCE> Zh. Anal. Khim. 31(4), 757-63 (Russ) J. Anal. Chem. USSR 31,
          621-6 (Eng)
<DATE> 1976

<ACCESSION NO.> 00*0000185      *******4
<AUTHOR> Thorsen, G.
<TITLE> Extraction and Separation of Metals Using Liquid Cation Exchangers
<SOURCE> S. African Patent No. 74 03,477
<DATE> Apr 1975
ENTER:
```

Figure 3. A specific search example.

<SEP SYS>

(Sep. System)

1 Adsorption	8 Electrolysis	27 Gradient	21 Sedimentation
2 Centrifugation	9 Electrophoresis	15 Ion Exchange	22 Solid-Gas
3 Chromatography	10 Electrostatic Ppt.	16 Liquid-Liquid	23 Solid-Liquid
4 Crystallization	11 Extraction	17 Magnetism	24 Solid-Solid
5 Diffusion	12 Filtration	18 Osmosis	25 Sublimation
6 Distillation	13 Flotation	19 Photolysis	26 Zone Refining
7 Electrodeposition	14 Gas-Liquid	20 Precipitation	

(*a*)

<INFOTYPE>

(Type of Info.)

1 Acidity effect	10 Decontamination factor	19 Matrix concn. effect	29 Synergism
2 Agent compn. effect	11 Device	20 Mechanism	30 Temp. effect
3 Agent concn. effect	12 Diluent compn. effect	21 pH effect	31 Thermodynamics
37 Agent stability	38 Flow rate effect	22 Pres. effect	32 Theory
4 Analytical method	13 Flowsheet	23 Process	33 Transferred sub. interaction use TSI
5 Antagonism	14 Intensive properties	39 Reagent loss	
6 At. no. effect	36 Interfacial phenomena	24 Review	
35 Bibliography	15 Isotherm	25 Sepn. degree	34 Valence effect
7 Capacity	16 Kinetics	26 Sep. sub. concn. effect	
8 Coefficient	17 Mathematical modeling	27 Solubility	
9 Constant	18 Matrix compn. effect	28 Stoichiometry	

(*b*)

<SEPAGENT>

(Separation Agent)

1 Acetylacetone	28 Hydrocarbon	97 Precipitant
2 Adsorbent	29 Hydroxamic acid	58 Primary amine
3 Alcohol	30 Hydroxyoxime	59 Pyrazoline
4 Aliphatic solvent	31 Inorganic acid	106 Pyrazolone
5 Alumina	32 Inorganic base	60 Pyridine
6 Amide	91 Inorganic compound	61 Pyrophosphate-org
7 Amine	Inorganic ion exchanger	62 Pyrophospho[illegible] acid-org
8 Amine oxid[illegible]	[illegible]propyltropolone	63 Pyrrolid[illegible]und
9 Anili[illegible]	52 [illegible]PT	64 Qu[illegible]pound
10 [illegible]N	53 Ph[illegible]	98 [illegible]mpound
[illegible]cycle-O	54 Phospi[illegible]	[illegible]ter
[illegible]eterocycle-S	55 Phosphoni[illegible]mpound	Xanthate
27 Heterocyclic compound	56 Phosphoric aci[illegible]	87 Zeolite
39 Hexone	57 Phosphorus ester	
use MIBK	105 Physical	

(*c*)

<MATRIX>

1 Acetate	13 Coal	25 Molten salt	37 Reductant
2 Acid	14 Complexant	26 Neutral	50 Residuals
3 Air	15 Cyanide	27 Nitrate	38 Resin
4 Alcohol	16 Fluoride	28 Nitrite	39 Salt
5 Ammoniacal	17 Formate	29 Ore	40 Silicate
6 Aqueous	18 Gas	30 Organic	41 Solvent refined coal
47 Base	52 Gel	49 Organic anion	use SRC
51 Biological medium	19 Glass	31 Oxalate	42 Sulfate
7 Borate	20 Glycolate	32 Oxidant	43 Sulfide
8 Brine	21 Halide	33 Oxide	44 Sulfite
9 Bromide	22 Iodate	34 Perchlorate	45 Tartrate
10 Carbonate	23 Iodide	53 Peroxide	46 Thiocyanate
11 Chloride	24 Lactate	35 Phosphate	
12 Citrate	48 Metal	36 Plastic	

(*d*)

Figure 4. A portion of the field and descriptor listings on the input form.

which a specific element is selected (or rejected) from a specific matrix. Combining the selection of one element with the rejection of another (or other) element(s) and a specific matrix will yield references, if any are in the data base, for the separation of *A* from *B* out of matrix *M*. An example of such a search is given in Fig. 3.

A variety of other search combinations can be done in a manner similar to the above. For example, separations possible for a given SEPARATION AGENT from a given MATRIX may be found by combining sets of appropriate terms from these two fields. References that list distribution coefficients for iron(III) between amine solutions and aqueous sulfate systems may be found by combining sets resulting from selecting "iron(III)" from SEPARATED SUBSTANCE, "amine" from SEPARATION AGENT, "sulfate" from MATRIX, and "coefficient" from TYPE OF INFORMATION. Other useful combinations will quickly become obvious to the user.

The same features of the data base that allow advantageous searching (i.e., categorization of index terms, precise indexing, and a limited scope) make indexing a research paper for the data base relatively simple. Indexer-abstractors are provided with a four-page form containing all the required index terms listed in the various fields plus space for bibliographic information and a short abstract. Listings of terms for some of the unique fields are shown in Fig. 4a-d, and the indexer is required only to highlight or circle appropriate index terms. Thus, inputting references is very rapid and simple. A manual containing instructions and definitions of terms is available for the use of indexer-abstractors.[2] Individual authors may thus easily (and accurately) abstract and index their own work for placement in the data base. Thus, this data base has the potential of becoming a means for those involved in any of several branches of separations science to keep in closer contact and to be more current with the work in their field of interest than is now possible. A further advantage is that the inclusion of the early, poorly indexed documents will prevent the repetition of work.

ACKNOWLEDGMENT

This research was sponsored by the Division of Chemical Sciences, U. S. Department of Energy under contract W-7405-eng-26 with the Union Carbide Corporation.

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1. U. S. Department of Energy Technical Information Center Publication No. DOE/TIC-4609, *Energinfo/On-Line, The DOE/RECON SYSTEM*, (February 1981).

2. J. W. Roddy, W. J. McDowell, and D. C. Michelson, *Separations Science Data Base: An Abstractor's Manual*, ORNL/TM-7805 (in press). [Available from: U. S. Department of Commerce, 5285 Port Royal Road, Springfield, Virginia 22161]