A Linear Line Notation for Flow Patterns in the Chemical Industry

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Flow patterns in the chemical industry consist of unit processes or unit operations which are sometimes highly interconnected. This paper describes a method for recording these flow patterns in a linear line notation for information retrieval purposes, using some of the basic principles of the DARC system. The notation is particularly adapted for both novelty and invention searches.

A. INTRODUCTION

The manufacturing of chemical products consists of combinations of unit operations and unit processes.[1] Unit operations are defined as those producing physical changes, such as mixing, separation, heating, grinding, etc.; unit processes as those producing chemical changes such as conversion or purification. In some chemical industries these unit processes and operations are often highly interconnected. The flow patterns involved in such processing are usually shown in the form of flow sheets. In the searches performed by Patent Offices it is often necessary to retrieve documents with a typical sequence of combinations of such unit operations or unit processes.

The field of petroleum refining serves as a good example for application of the method to be described, but it can also be applied to other fields where the sequence of operations is of importance.

Documents dealing with the production of petroleum products often describe a complicated interconnection of cracking, reforming, hydrogenation, and other processes with distilling, mixing, extraction, or other operations. Recycling and bypassing are also frequently involved.[2]

A search for a specific sequence of units in such documents is generally rather difficult and time consuming. A hierarchical classification system such as the International Patent Classification or the U.S. Patent Office classification provides only for entries dealing with a process or operation unit in itself, and possibly for a few combinations of such units without mention of their sequence (e.g., International Patent Classification (2nd ed) C 10 G 34/00, 37/00, and 39/00) or, only very broadly (e.g., U.S. class 208/49 to 208/105). In existing computer search systems, the recording and retrieval of such data are usually based on indexing the processes as such, post-coordinate search questions allowing detection of the presence of these units.

Methods exist for the storage and retrieval of more precise information, i.e., information relating not only to the kind of unit process and operation involved, but also to the interconnection between these units and to the kind of product flowing from one unit to another. Such a method has been described for the field of petroleum refining using 80 column punch cards implemented on mechanical sorters (3). Moreover, the TOSAR system developed by Fugmann et al. also deals with this kind of information which is recorded by means of graphs and searched using a specially developed computer program.[4] A method of recording a sequence of unit processes or unit operations in a code sentence has also been described by Meyer.[5]

In this paper an attempt is made to record a pattern in a linear line notation in a way easy to record and to retrieve by using some of the basic principles of the DARC system.[6] Linear line notations are widely used in the field of organic chemistry and the two-dimensional (sometimes even three-dimensional) recording and searching of organic compound structures is well known,[7] but most of these line notations are specially adapted for and are limited to chemical compounds. Consequently the search programs used in these systems are inadequate for the notation and retrieval of concept linkage.[8]

B. DARC SYSTEM[6]

The DARC system was developed by Professor Dubois of the University of Paris, and concerns a system for *D*ocumentation and *A*utomation of searches ("*R*echerches") by *C*orrelation, reflecting both the positional and topological properties of the entities concerned.

Although this system is implemented mainly for the recording of organic chemical compounds, its application is not limited to this particular field. It can be applied to other subject matter, in which both topological and positional properties are of importance.[9]

Briefly, the structure of an organic compound is recorded by starting from a focal point and by representing the surrounding environment in a series of concentric circles. The elements on these circles and their mutual links are numbered, put in matrix form, and computed to a linear notation. After recording the focal point the elements on the first two concentric circles are computed. Each of the elements on the second circle is then taken as a new focal point to compute the data on the following two concentric circles, and so on.

Although it would be possible to record flow patterns linearly by direct application of the rules of the DARC system, the present intention is to develop a method specially adapted to this particular field, involving some modifications of the rules of the DARC system. This method certainly has the drawback that most of the algorithms of the DARC system also have to be modified, but on the other hand the adapted algorithms are more suitable to the task in hand and lead to simplification of search strategy. The latter is of importance for patent searches in this field, in order to retrieve the relevant state of the art.

C. CODING OF THE TOPOLOGICAL INFORMATION

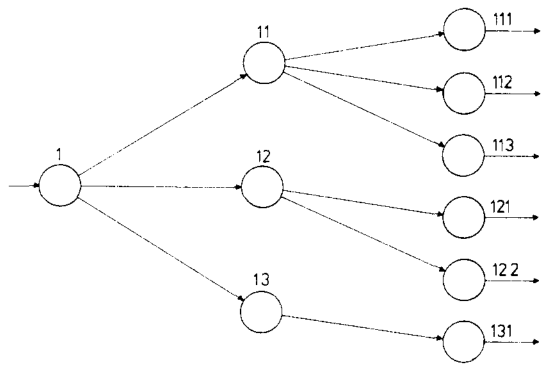
The topological information is recorded by using as a focal unit (i.e., as starting point) the unit to which the feed is added. Starting from this focal unit, all other units are recorded successively. First those directly linked to the focal unit (termed first order units) are dealt with, then those linked to the first-order units, i.e., second-order units, etc. In other words, each unit successively plays the role of a focal unit. The system is, in its operation, analogous to a wave which begins at the focal unit and moves outward over the flow sheet in the direction of the flow.

The focal unit is indicated by a single digit. First-order units are indicated by two digits, in which the first is the digit assigned to their focal unit. Second-order units are assigned three digits of which the first two indicate the first-order unit with which it is directly linked, and so on.

Table I

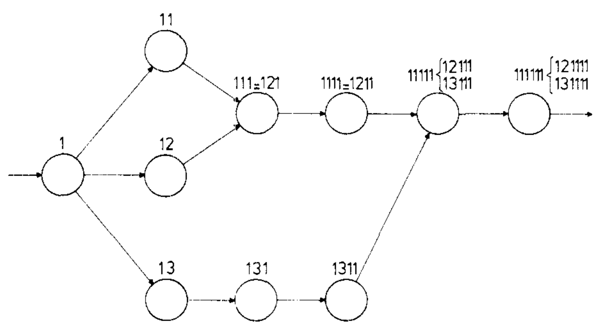
Products		Units	
Crude	= RO	Atmospheric distillation	BDA
Light naphtha	= NW	Distillation and stripping	BDS
Heavy naphtha	= NX	Thermal reforming	RTT
Diesel oil	= OW	Fluid cracker	CCF
Residue	= RA	Regenerator	SCF
Cracked naphtha	= NC	Mixing	OMX
Cracked gasoil	= OC		
Fresh catalyst	= SL	Reformer outlet	UR
Dirty catalyst	= SM	Cracker outlet	UC
Gasoline	= NM		

The numbered units are regarded linearly in the sequence of their numerical value. Each unit is placed in parentheses to form a unit block, which shows clearly that it is an entity in itself and which allows the addition (in each block) of extra information concerning that unit.



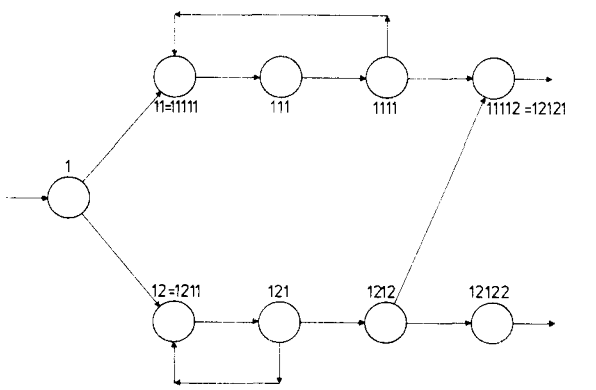
(1)(11)(12)(13)(111)(112)(113)(121)(122)(131)

Coinciding Units. When a unit is connected to two units of a higher order, the unit will have two different numerical identities; i.e., two flows are added to the same unit. This is shown via an indication of equality between the two numerical identities:



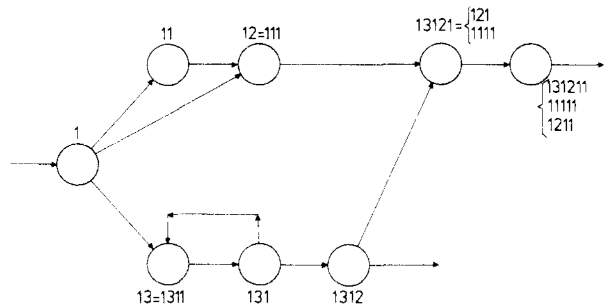
(1)(11)(12)(13)(111 = 121)(131)(1111; 1211)(1311)(11111; 12111 = 13111)(111111; 121111; 131111)

Recycling. When feeds are recycled, the flow is from a unit of a lower order to a unit of a higher order. In this case the same principle is applied as was explained for coinciding units.



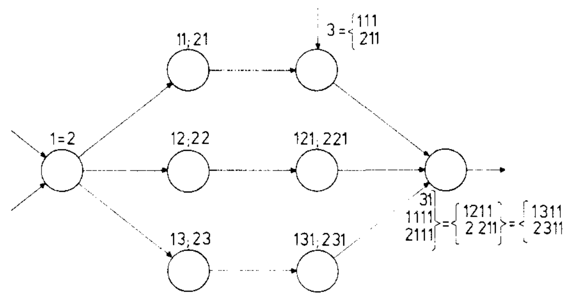
(1)(11 = 11111)(12 = 1211)(111)(121)(1111)(1212)(11112 = 12121)(12122)

Bypassing. A unit is connected to a second unit by two flows, one direct and one passing via a third unit. This case can be considered identical with that of coinciding units, i.e., a unit of higher order coincides with a unit of lower order.



(1)(11)(12 = 111)(13 = 1311)(131)(13121 = 121; 1111)(1211; 11111; 131211)(1312)

Several Feeds. Often, in chemical processes, several feeds are added together simultaneously. Units to which outside feeds are added are all considered as focal units and are treated accordingly for numbering purposes.



(1 = 2)(3 = 111; 211)(11; 21)(12; 22)(13; 23)(31; 1111; 2111 = 1211; 2211 = 1311; 2311)(121; 221)(131; 231)

D. CODING OF POSITIONAL INFORMATION

In addition to the flow pattern, i.e., the topological information, a chemical flow sheet also shows the unit processes or operations applied, the materials added, and the products made, i.e., positional information.

The topological information is coded by means of a numerical identification indicated in a unit block, one unit block being present per unit process or operation. These unit blocks may also be used for recording the positional information.

Unit Process/Unit Operation. The unit process or operation is shown in the unit block after the numerical identification *and* separated from the latter by a slash. By means of a term list or thesaurus, all unit operations or processes of importance can be shown. For example, a three-letter code could be used for identifying the process or operation. The first letter indicates the genus (e.g., cracking, C--; re-forming, R--), the second letter the species (e.g., CT- for thermal cracking, CC- for catalytic cracking), and the third the subspecies (e.g., CCF for fluid catalytic cracking, CCH for Houdry catalytic cracking, CCA for undefined catalytic cracking).

It would be possible to provide still more information about the unit process or apparatus shown by this three-letter code, such as reaction temperature, pressure, catalyst. This information could be recorded in a specified sequence after the three-letter symbol of the unit e.g., (.../CCF, 400–500 °C, 1–3 atm, Al_2O_3–SiO_2).

Materials. A numerical identification in a unit block defines the links with the units of higher order or focal unit, i.e., the material flowing from a unit of higher order or focal unit to that unit. Each numerical identification in a unit block stands for a material added to that unit. Therefore the materials are marked directly after the numerical identification to which they are related. The material is recorded by means of a term list or thesaurus. For example, a two-letter code could be used for showing all materials of importance in that art. The first letter will indicate the genus (A- for alkanes, N- for naphthas, R- for residue fraction) and the second the species (NC for cracked naphtha, NV for virgin naphtha, NR for regular gasoline, NA for naphtha or gasoline in general).

Here also more information about the product can be given, if desirable, such as boiling range, viscosity, etc., by a separate recording after the two-letter product code, e.g., (*a*...*f*NC, *b*.80–100 °C/...).

Products. Products are considered to be materials withdrawn from the flow sheet. Materials withdrawn from a flow sheet are marked in a unit block, and the numerical identification will show the flow withdrawn. These materials can be one of the following.

(1) Materials for which it is mentioned (but not shown) on the flow sheet that they will be processed further on. This case is treated in a similar way to the processes indicated on the flow sheet, e.g., a document mentioning, but not showing it on the flow sheet, that a light virgin naphtha fraction is withdrawn and that further on it may be mixed with other naphtha fractions is given as $(a_1b_1...\mathrm{NW} = a_2b_2...\mathrm{NA/OMX})$; the small letters *a*, *b*, ... represent digits.

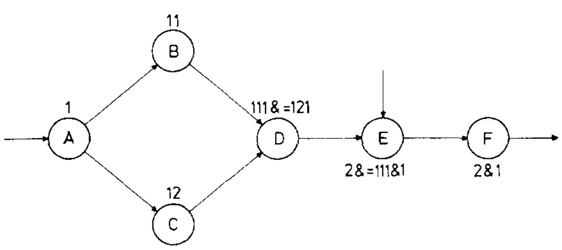
(2) Materials which are considered to be waste (*waste products*), e.g., waste water, solvent, etc. In this case a minus sign is indicated in the unit block after the slash; e.g., steam is released from a unit (*abc*...*m*GS/−).

(3) Final products: in this case an asterisk is shown after the slash. It is also suggested that a two-letter code be used for indicating a final product, thus NR for regular gasoline, NP for jet fuel, etc.; for instance, if a flow of jet fuel is produced: *ab*...*m*NP/*).

E. THE AMPERSAND

When a unit in a unit block has more than one numerical identification due to different inlets to that unit (e.g., coinciding units, bypassing, recycling), several cases must be considered.

(1) The different identifications are due to inlet flows, the products of which will be processed in the successive units of lower order. These successive units are identified by placing digits after the lowest of the identification numbers marked in said unit block. However, an ampersand is put after this lowest number to show in the first unit block that this number will be used for marking the successive units and to indicate that this identification number with ampersand has to be replaced in all other unit blocks by all of its assimilated numbers of the first unit.



(1/A)(2& = 111&1/E)(11/B)(12/C)(2&1/F)(111& = 121/D)

which should be read out completely

(1/A)(2 = 1111/E)(11/B)(12/C)(21/F)(111 = 121/D)

or

(1/A)(2 = 1211/E)(11B)(12/C)(21/F)(111 = 121/D)

or

(1/A)(2 = 1111/E)(11/B)(12/C)(11111/F)(111 = 121/D)

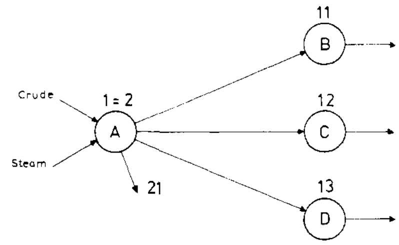
or

(1/A)(2 = 1211/E)(11/B)(12/C)(1211/F)(111 = 121/D)

When determining the sequence of numbering, the ampersand is neglected. Thus 1&2 follows 11 when coding.

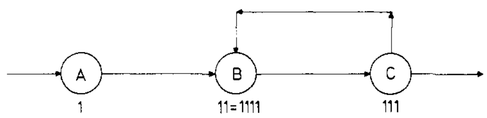
(2) One of the identification numbers is derived from a product which is added only temporarily and thus has no direct influence on the successive units of higher order.

In this case the ampersand is not used, e.g.,



(1 = 2/A)(11/B)(12/C)(13/D)(21/−)

(3) One of the identification numbers is derived from a recycle flow. In this case also, the ampersand is not used.

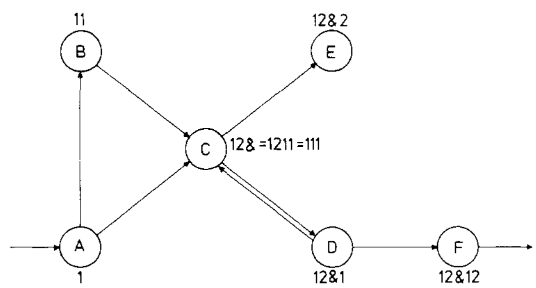


(1/A)(11 = 1111/B)(111/C)

If one were to write (11& = 11&11), then 111 would become 11&1 and thus 11&111, 11&11111, etc., which becomes endless.

This is understandable, since recycling implies that a part of the product is recycled either for further conversion, or to regulate the temperature, or to be used as an auxiliary material (solvent catalyst), or as a reagent (hydrogen).

Special Cases. (a) There are other effluent flows from the unit to which a product flow is recycled. In this case the ampersand is used for identifying all relevant units in all the successive steps, but the ampersand is deleted in the identification number of the recycle flow itself.



represents

(1/A)(11/B)(12& = 111 = 1211/C)(12&1/D)(12&2/E)(12&12/F)

which represents:

(1/A)(11/B)(12 = 111 = 1211/C)(121/D)(122/E)(1212/F) or
(1/A)(11/B)(12 = 111 = 1211/C)(1111/D)(1112/E)(11112/F) or
(1/A)(11/B)(12 = 111 = 1211/C)(12111/D)(12112/E)(121112/F)

(b) A flow is added to the recycle stream. In this case the ampersand is used, except for the identification number of the

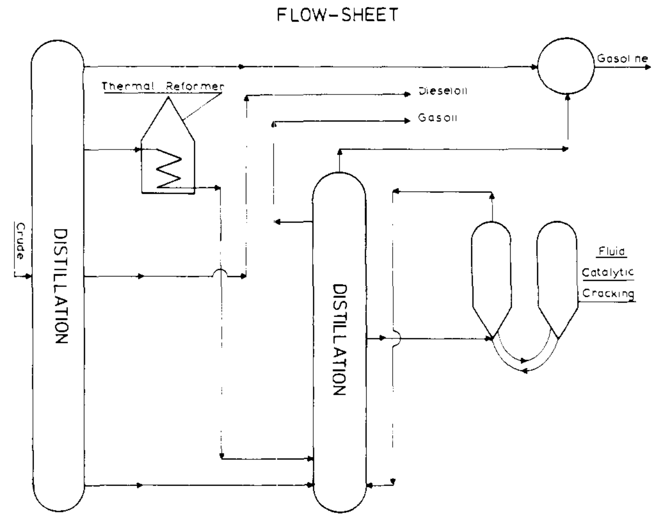


Figure 1. A petroleum refinery flow-sheet.

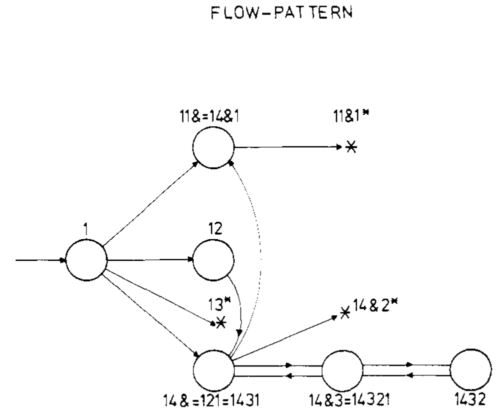
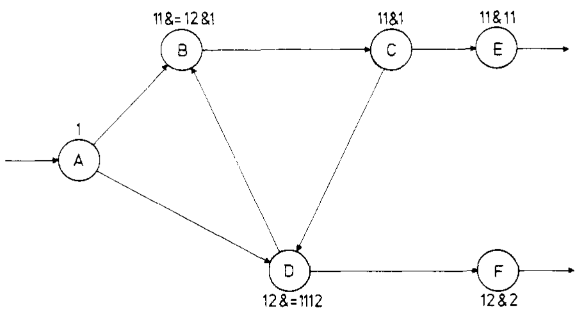


Figure 2. Flow-pattern.

recycle flow itself, where it is omitted.



(1/A)(11& = 12&1/B)(12& = 1112/D)(11&1/C)(12&2/F)-(11&11E)

which represents

(1/A)(11 = 121/B)(12 = 1112/D)(111/C)(122/F)(1111/E)

or

(1/A)(11 = 11111/B)(12 = 1112/D)(1211/C)(11112/F)(12111/E)

or

(1/A)(11 = 11111/B)(12 = 1112/D)(111111/C)(11112/F)-(1111111/E)

The last of the above alternatives shows, in fact, that a recycled product has been processed in the other successive units. This information may be useful, since in this case the recycled flow has itself gone through a further process or operation.

Avoidance of a Common Pitfall. In order to avoid "loops", i.e., closed circuits in the notational logic, the digits placed before an ampersand in an identification must never, whether directly or indirectly, be placed in an equality relationship with another identification having the same digits. Thus, never put:

$-.a_1b_1c_1...m_1\& = a_1b_1c_1...m_1\&n_1p_1$

or

$-a_1b_1c_1...m_1\& = a_2b_2c_2...m_2\&n_2p_2$ and $a_2b_2c_2...m_2\& = a_1b_1c_1...m_1\&n_1p_1$

F. NUMBERING SEQUENCE

The numbering sequence assigned to the units of a given order is unimportant and has no influence on retrieval. However, in order to obtain a uniform line notation, it is desirable that a given flow sheet should be coded in a standard way; i.e., the same unit should receive the same identification independently of the analyzer. The numerical identification alloted to a unit shows its link with the preceding unit, i.e., the unit of higher order. It is composed of the digits of this unit of higher order followed by a digit indicating the units to which its effluents are added. It is suggested that this digit should be in the order of the molecular weight of said effluent products. Alternatively, to allow automatic coding of the graph, it may be better to use the topological characteristics of the graph as criteria, e.g., first the less branched, shorter and less complicated flowstream.

G. EXAMPLE

For an example, see the flow-sheet in Figure 1 and corresponding Table I for the flow-pattern in Figure 2. The linear notation becomes:

(1RO/BDA)(11&NW = 14&1NC/OMX)(12NX/RTT)(130W/*)
(14&RA = 121UR = 1431UC/BDS)(11&1NM/*)(14&20C/*)
(143RA = 14321SL/CCF)(1432SM/GCF)

H. RETRIEVAL

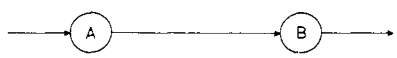
This notation system is particularly adapted for both novelty and invention searches. By a proper choice of the genus and species marks for products and unit processes or operation, browsing will be easily possible.[10] A search question can first be put in its most specific form, and, if no proper response is obtained, it can be broadened to the most general form which may still be of interest.

Also the number identifications of a unit process or operation show the complete backflow of the feed to that unit. This allows searches on all downstream or upstream processes or operations; for a downstream process or operation only the beginning of the number identification should coincide, and for an upstream process or operation the number identification should contain the same initial digits.

I. SEARCH STRATEGY

In the examples given below, the letter symbols *a b c ... m* represent digits from the numerical identity of the unit in sequential order.

(1) Units in Series. a. In straight sequence:

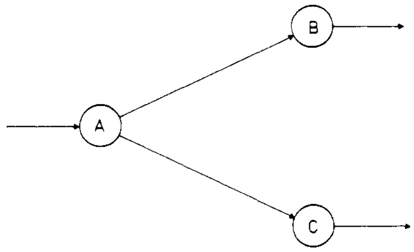


Algorithm
$(a_1b_1c_1...m_1/\mathrm{A}) + (a_1b_1c_1...m_1n/\mathrm{B})$

b. With one or more interjacent units:

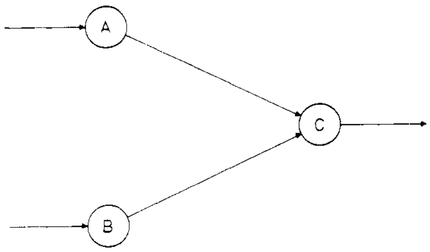
Algorithm
$(a_1b_1c_1...m_1/\mathrm{A}) + (a_1b_1c_1...m_1np...qr/\mathrm{B})$
$np...q$: represents the number of interjacent units

(2) Units in Parallel. a. With flow from the same unit:



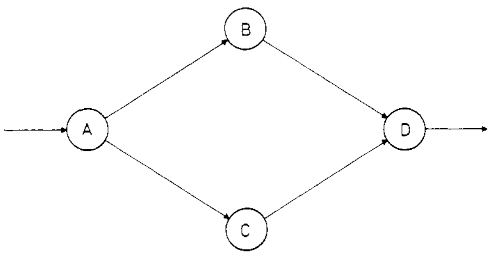
Algorithm
$(a_1b_1c_1...m_1n_1/\mathrm{B}) + (a_1b_1c_1...m_1n_2/\mathrm{C})$

b. With flow to the same unit:



Algorithm
$(a_1b_1c_1...m_1n_1 = a_2b_2c_2...m_2n_2/\mathrm{C})$

c. With flow from and to the same units:

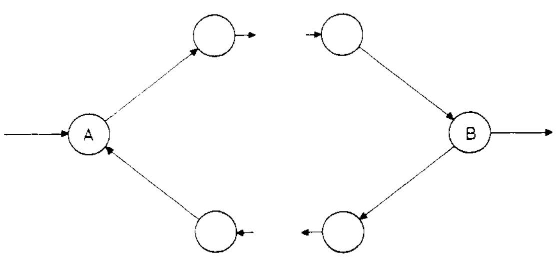


Algorithm
$(a_1b_1c_1...m_1n_1...q_1 = a_1b_1c_1...m_1n_2...q_2/\mathrm{D})$

(3) Recycling. a. Directly from one unit to another:

Algorithm
$(a_1b_1c_1...m_1 = a_1b_1c_1...m_1np/\mathrm{A}) + (a_1b_1c_1...m_1n/\mathrm{B})$

b. With adjacent units:

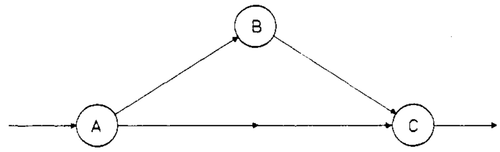


Algorithm
$(a_1b_1c_1...m_1 = a_1b_1c_1...m_1n..pq...r/\mathrm{A}) + (a_1b_1c_1...m_1n...p/\mathrm{B})$

Table II

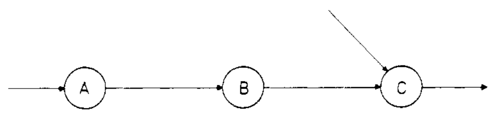
$(a_1...f_1\,\mathrm{NW}/\alpha\alpha\alpha)$	:	$(11\&\mathrm{NW}/\alpha\alpha\alpha)$	
$(a_2...f_2\alpha\alpha/\mathrm{RTT})$	:	$(12\alpha\alpha/\mathrm{RTT})$	
$(a_3...f_3\alpha\alpha/\mathrm{CCF})$	:	$(14\&3\alpha\alpha/\mathrm{CCF})$	
$(a'...f'...\mathrm{NM}/*$	:	$(11\&1\mathrm{NM}/*)$	
$(a'...f'...\alpha\alpha = a''...f''...\alpha\alpha/\alpha\alpha\alpha)$	:	$(11\&\alpha\alpha = 14\&1\alpha\alpha/\alpha\alpha\alpha)$	$11\&\alpha\alpha = 14311\alpha\alpha$
$(a'...f'...\alpha\alpha = a'''...f'''...\alpha\alpha/\alpha\alpha\alpha)$	:	$(121\alpha\alpha = 1431\alpha\alpha = 14\&\alpha\alpha)$	$1211\alpha\alpha$
			$141\alpha\alpha$

(4) Bypassing



Algorithm
$(a_1b_1c_1...m_1/A) + (a_1b_1c_1...m_1n_1/\mathrm{B}) + (a_1b_1c_1...m_1n_2 = a_1b_1c_1...m_1n_1p/\mathrm{C})$

(5) Several Feed Inlets



Algorithm
$(a_1b_1c_1...m_1n_1p = a_2/\mathrm{C}) + (a_1b_1...m_1n_1/\mathrm{B}) + (a_1b_1...m_1/\mathrm{A})$

J. A WORKED-OUT EXAMPLE OF SEARCH STRATEGY

Question: Process to prepare regular gasoline by mixing a fluid, catalytically cracked naphtha, a pipe still thermally re-formed naphtha, and a light virgin naphtha.

Symbols (see Table I)

Regular motor gasoline NM
Re-formed naphtha NR
Cracked naphtha NC
Light virgin naphtha NW
Mixing operation OMX
Fluid catalytic cracking CCF
Pipe still thermal re-forming RTT
Atmospheric distillation BDA
The symbol α stands for any capital letters from A to Z.

(1) Precise Question:

$$(a_1b_1...m_1\mathrm{NM}/*) + (a_1b_1...(m-1)\mathrm{NW} = a_2b_2...f_2\mathrm{NR} = a_3b_3...f_3\mathrm{NC}/\mathrm{OMX})$$
$$+ (a_2b_2...(f_2-n)\alpha\alpha/\mathrm{RTT}) + (a_3b_3...(f_3-n)\alpha\alpha/\mathrm{CCF})$$

(n being 1 or 2)

(2) Browsing. If there is no response to this precise question, we can broaden the search question in different ways:

(1) By browsing in the kind of process involved, e.g., instead of CCF (fluid catalytic cracking), CCA (unspecified catalytic cracking) or even CC- (any catalytic cracking) can be taken. Similarly RTT can be replaced by RTA (unspecified thermal re-forming) or even RT- (any thermal re-forming).

(2) By browsing in the kind of products, e.g., NM could be replaced by NP (premium gasoline).

(3) By browsing in the flow pattern. It could be that two of the three fractions were already mixed in an earlier operation step. So a more general search question may be

considered of importance. For example:

$$(a_1 \ldots f_1\text{NW}/\alpha\alpha\alpha) + (a_2 \ldots f_2\alpha\alpha/\text{RTT}) + (a_3 \ldots f_3\alpha\alpha/\text{CCF})$$
$$+ (a' \ldots f' \ldots \text{NM}/*) + (a' \ldots f' \ldots \alpha\alpha = a'' \ldots f'' \ldots \alpha\alpha/\alpha\alpha\alpha)$$
$$+ (a' \ldots f' \ldots = a''' \ldots f''' \ldots \alpha\alpha/\alpha\alpha\alpha)$$

$a'..f'...$; $a''..f''...$; or $a'''..f'''...$ being $a_1..f_1...$; $a_2..f_2...$; or $a_3..f_3...$. The flow pattern described in Figure 2 would respond to this search question, the block correspondence in Table II being found in the linear line notation.

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NEWS AND NOTES

BOOK REVIEWS

Computer-Readable Bibliographic Data Bases. A Directory and Data Sourcebook. Compiled and edited by MARTHA E. WILLIAMS and SANDRA H. ROUSE, American Society for Information Science, Washington, D.C. 1976. 814 pp. $68.00.

This directory of 301 data bases is an update of the 1973 "Survey of Commercially Available Computer-Readable Bibliographic Data Bases", edited by J. H. Schneider, M. Gechman, and S. E. Furth, which reported on 81 data bases. A growth rate of 370% in three years is quite phenomenal and certainly justifies the production of the new edition in a three-ring binder with $8^1/_2 \times 11$ pages for updating on a six-month schedule for the data bases and annually for the indexes.

Information on each data base includes the following if applicable or available: data base name, producer, distributor, generator, availability, size, frequency, scope, subject matter, document types covered, data elements, etc. There are four indexes: subject category; name/acronym/synonym; producer; and processor. Each data base description begins on a new page and is assigned as many pages as required but without page numbers. Entries are arranged alphabetically by the data base acronym, such as ABIPC for "Abstract Bulletin of the Institute of Paper Chemistry".

There are 91 data bases listed in the index under Chemistry and Chemical Engineering, almost one-third of the total. There is no entry for Market Information. Although considerable information is given for each data base, the kind of information that enables a user to evaluate value is missing. The directory will be most meaningful to producers and processors and least valuable to users.

Cumulative Index to Volumes 1–10, Annual Review of Information Science and Technology, 1966–1975. Edited by J. L. HARRIS, P. L. ASKEY, and C. HINDELS, American Society for Information Science, Washington, D.C. 1976. viii + 215 pp. $27.50.

This cumulative index to the first ten volumes of ARIST, as the series is commonly called, is an update and continuation of the one published in 1972 covering the first seven volumes. The indexing by subject and names is thorough and easy to use, especially with the employment of running heads at the top of each page. See references, especially for acronyms, are plentiful and helpful to the user.

NEWS ITEMS

Mass Spectral Data

The U.S. Environmental Protection Agency has contracted with the American Chemical Society's Chemical Abstracts Service to produce a Mass Spectra Handbook corresponding to the content of the EPA/National Institutes of Health machine-readable mass spectral data base. The handbook will contain mass spectra for approximately 30 000 substances along with the substances' structure diagrams, names, molecular formulas, molecular weights, and CAS Registry Numbers. It will include previously unpublished mass spectral data.

The handbook will be compiled and organized entirely by computer and composed through CAS's computer-directed photocomposition system. Mass spectra in the handbook will be generated and photocomposed from computer-readable data provided by EPA. Names and molecular formulas will be extracted automatically from the CAS Chemical Registry System, and most structure diagrams in the handbook will be generated algorithmically from connection table records stored in the CAS Registry files.

The handbook is being produced by CAS under an extension of a contract with EPA's Management Information and Data Systems Division under which CAS has been registering chemical substances in various data files, including the mass spectral data base, and providing Registry Numbers, names, and connection tables for use in the NIH/EPA Chemical Information System. CAS has registered approximately 100 000 substances for EPA under this contract since 1974.

Symposium on Patent Information

The German Society for Documentation (Committee for Patent Documentation (DGD/APD) and the German Patent Office (DPA) in cooperation with the World Intellectual Property Organization (WIPO) will organize an International Symposium on Patent Information and Documentation, at the Sheraton Hotel, Munich, from May 16 to 18, 1977.