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A Unified Method of Delineating Polymeric Species*

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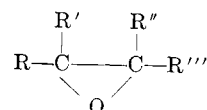
Much work is currently being done in the field of data handling as applied to chemistry. There is obviously a great need for methods of organizing, manipulating, storing, and retrieving chemical data. One of the areas in which many chemical data are being generated and which is particularly difficult to systematize is the field of polymer chemistry. The problem of an unambiguous method for encoding chemical formulas for machine handling is far from solved. The problem of delineating individual members of a polymeric series has hardly been considered.

The need for a method of organizing and delineating polymeric species is particularly apparent to one who reads the patent literature. Hundreds of patents are being issued on uses for, methods of making, or compositions of matter involving polymers. It is becoming increasingly difficult to determine the scope of claims, or the novelty of particular compositions. This paper presents a method of defining polymeric species, and of differentiating between species and between individual members of a species. The method has been applied with particular success in the field of oxyalkylates but is sufficiently general to be applicable to many if not most fields of polymers.

In the mathematical discussion of the development and use of this method, specific examples will be taken almost solely from the alkylene oxide polymers and for this

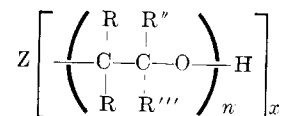
reason a brief discussion of the chemistry of this class is given.

Alkylene oxides have the general formula



where R, R', R'', and R''' may be, for example, hydrogen, an aliphatic radical, a cycloaliphatic radical, an aryl radical, etc. The R's may also be joined to form a cyclic structure. In cases where one or more of the R's contain an epoxide group, a diepoxide or a polyepoxide results. For the purposes of simplicity this discussion will consider only the materials with one epoxide group.

Alkylene oxides react with active centers of other organic or inorganic molecules to build up polyether chains of considerable length. The generic reaction product may be written:



where n is the number of monomer units in the chain and x is the number of reactive sites in the starting molecule.

The relative reactivity of the chain terminal groups and of the original reactive sites with respect to the monomer determines the positions and relative lengths of

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the chains. In almost all reactions of this type it is understood that a single pure compound is not produced. The reaction product is a "cogeneric mixture."

In dealing with polymeric reactions of this type mathematically, it is possible to break the procedure into several distinct operations, as:

1. Designation of starting material
2. Designation of reaction conditions
3. Step-wise reaction of monomer with starting material
 - a. Selection of monomer composition
 - b. Specification of number of units of monomer to be reacted with starting material

The product resulting from step 3 above can then be used as the starting material for a new family of polymers by repeating steps 2 and 3. This procedure can be repeated as often as desired. Each of the three above steps will now be discussed separately and certain terms defined.

1. Designation of starting material. Mathematically this operation consists of selecting a member S_x , from the class of all materials or mixtures that are susceptible to oxyalkylation. These materials may be said to constitute a class, $S_1, S_2, S_3, S_4, \dots, S_x, \dots, S_n$ where the subscript refers to the chemical identity of the starting material. Examples of subclasses of this large class are alcohols, amines, carboxylic acids, phenols, mercaptans, etc.

2. Designation of reaction conditions. It is known that the type and amount of catalyst, the temperature, pressure, rate of addition, and other factors may affect the composition of the final reaction mixture. For this reason it is necessary to specify the values of any parameters that can affect the course of the reaction. This is mathematically equivalent to selecting a function $F_x(T, P, c, \dots)$ from a general class of all possible conditions.

3. Stepwise reaction of monomer with S_x , under conditions F_x .

- a. Selection of monomer composition

The three most common 1,2-alkylene oxides are ethylene oxide, propylene oxide, and butylene (1,2- or 2,3-) oxide. Also known are other mono-oxides such as octylene oxide, styrene oxide, cyclohexene oxide, etc., and also di- and poly-epoxides.

These materials constitute a class: $M_1, M_2, M_3, \dots, M_x, \dots, M_n$. In the non-limiting case, any or all of the members of the class may be used singly or in combination to constitute the monomer mixture. In most cases a single monomer is used; however, mixtures of two monomers have been used. The commercial butylene oxide is usually a mixture of the 1,2- and 2,3-isomers. For purposes of illustration, most of the following examples will deal with either ethylene oxide (EtO), propylene oxide (PrO), butylene oxide (BuO) with specific reference to the 1,2-isomer in commonly available technical pure form unless otherwise specified, or mixtures of these monomers. The monomer composition can be represented symbolically thus:

$$O(aM_1, bM_2, \dots, yM_x)$$

where O represents the polymerization steps and M_1, M_2, \dots, M_x are the monomers in the mixture and a, b, \dots, y are the proportions of each monomer. It follows that if

the indices a, b, \dots, y are expressed as weight or mole percentages, then $a+b+\dots+y = 100$, and if the indices are expressed as decimal fractions then:

$$a+b+\dots+y = 1$$

Specifically if only ethylene oxide were used the notation would be M(EtO). If equal weights of ethylene and propylene oxide were mixed to form the monomer mixture the notation could be M(0.5 EtO, 0.5 PrO w/w) where the indices are expressed as weight fractions. If equal moles of the two pure monomers were mixed then the designation could be M(0.5 EtO, 0.5 PrO m/m). These two mixtures are obviously different. A simple mathematical calculation will show that M(0.5000 EtO, 0.5000 PrO m/m) is equivalent to M(0.4314 EtP, 0.5686 PrO w/w).

- b. Specification of number of units of monomer (M_x) to be reacted with S_x, F_x .

It now remains only to specify how much monomer should be allowed to react with the starting material. There are several units that can be used but the most common are weight of monomer per unit weight of S_x , moles of monomer per mole of S_x , and percent M_x in final product. Each of these has certain advantages and disadvantages. I prefer to express the amount of monomer or monomer mixture as moles of equivalent epoxide per mole of S_x . In the case of single or mixed monoepoxide monomers this is numerically equal to moles of monomer per mole of starting material.

On the basis of the above discussion it is now possible unambiguously to specify the composition of any particular oxyalkylation product in terms of the starting material, conditions, and kinds and amounts of monomer used. The general notation is:

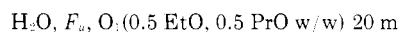
$$S_x, F_x, O_1(aM_1, bM_2, \dots, yM_x)N_1, \\ O_2(a'M_1, b'M_2, \dots, yM_x)N_2 \\ \dots \dots O_n(a_nM_1, b_nM_2, \dots, y_nM_x)N_n$$

where O_1, O_2, \dots, O_n represent successive oxyalkylation steps and N_1, N_2, \dots, N_n are the amounts of oxide added at each step. As a specific example of this notation may be cited the material covered in U. S. Patent 2,674,619 to Lundsted and now sold commercially by the Wyandotte Chemical Company under the trade name Pluronic L-64. This material, according to the manufacturer, is made by adding ethylene oxide to a polypropylene glycol of molecular weight 1750 until the ethylene oxide portion represents 40% of the weight of the final molecule. In the above notation this material is regarded as the two-step reaction product, where S_x is water, which is then allowed to react first with propylene oxide then with ethylene oxide. A polypropylene glycol of molecular weight 1750 is equivalent to adding about 30 moles of propylene oxide to one of water. If this represents 60% of the final molecular weight, the final molecular weight will be about 2900. This would require the addition of about 26 moles of ethylene oxide to the polypropylene glycol to produce the final product. Thus the notation would be:

$$H_2O, F_p, O_1(\text{PrO } 100\% \text{ m}) 30.17, O_2(\text{EtO } 100\% \text{ m}) 26.51$$

where F_p represents the reaction conditions as specified in the above-cited patent.

Another example is the material described in U. S. Patent 2,425,845 to Toussaint, *et al.*, and sold commercially by Carbide and Carbon Chemical Company as Ucon 50HB 260. This material is made by treating one mole of water with about 20 moles of a mixture of ethylene oxide and propylene oxide containing equal weights of each oxide. It is made by a one-stage process and the notation is:



where F_u refers to the reaction conditions of the patent. Note that the units in which the mixture is expressed are indicated by w/w to show a weight ratio and that the amount added is expressed as 20 m to show that it is expressed in moles. Obviously, the units in which either the mixture ratio or the amount added could be changed without affecting the identity of the notation.

It should be clear that the above-described notation will unambiguously delineate any possible polyalkylene glycol polymer. It is not, however, in itself, useful in developing a meaningful picture of the whole field.

The procedure described in this paper consists of a mapping technique wherein a suitable composition space is chosen and properties of members of a class of polymers are mapped in the space in such a way that their interrelationships are readily displayed. Mathematically this amounts to establishing a one-to-one correspondence between the individual members of a class of polymers and the individual points in an appropriately chosen composition space. For instance, all the possible mixtures of methyl alcohol and water can be represented by points on a line segment such as Fig. 1. In Fig. 1, A represents pure methanol and B represents pure water. The point, P, represents a mixture of water and methanol. The location of point P is determined by the proportions of the two compounds in the mixture. As point P approaches A the mixtures represented become richer in methanol. This particular composition space is one-dimensional, unambiguous, definitive, and commutative. It represents all possible mixtures, each point represents one and only one mixture, and each mixture can be made either by adding water to methanol or methanol to water. Mathematically this is the same as saying that point P may be approached from either direction without changing its meaning.

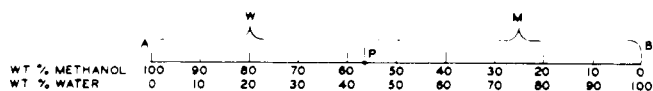


Fig. 1.

When the order in which a sequence of operations is performed affects the final result, the system is said to be non-commutative. The spaces employed in this method will, for the most part, be non-commutative. In many organic chemical syntheses the order in which the steps are performed determines the product obtained. Thus, it is clear that if one treats one mole of water with five moles of ethylene oxide and then with five moles of propylene oxide one obtains a different material from that if one treats one mole of water first with five moles of propylene oxide and then with five moles of ethylene oxide.

The appropriate composition space for the polymeric species under consideration is characterized as:

1. S_x and F_x serve as indices to differentiate individual composition spaces which are otherwise mathematically identical.
2. The spaces are fundamentally non-commutative in that each of the dimensions making up the space must be traversed in the designated sequential order.
3. Dimensional segments of the composition spaces are of two kind, "selection figures" where the monomer composition is specified, and "polymerization figures" where the amount of monomer is specified. In general, the non-commutative aspects of the space require traverse alternately through first a selection figure, then through a polymerization figure.
4. The composition space contains one selection figure and one polymerization figure for each successive different oxyalkylation step required to produce the particular molecular species.

The one-component polyglycols afford a good example of classes that are easily displayed in one-dimensional, non-commutative diagrams. Fig. 2 shows a group of such composition spaces. Fig. 2-1 could be used to represent the class of polyethylene glycols. In this case the starting material is water and the synthesis of any member of the class is a one-step process consisting of the addition of the desired amount of ethylene oxide under the appropriate conditions. Each point on the line represents a possible cogeneric mixture resulting from a reaction of this kind. All possible products can be represented by extension of the line to the right. If a reaction technique were to be used which resulted in pure compounds rather than mixtures, a non-continuous space such as Fig. 2-6 would be used to display the class since theoretical compositions with fractional mole additions would be impossible. In cases where cogeneric mixtures occur the number of moles added per mole of starting material is plotted and the distribution of actual species in the mixture is assumed to be set by F_x . The "selection figure" in these cases is the initial point of the line. The rest of the line constitutes the "polymerization figure."

Figures 2-2 and 2-3 could be used to display polypropylene glycols and polybutylene glycols. They differ from each other and Fig. 2-1 only in the selection figure point which represents a different reactive monomer. If a different starting material, *e.g.*, an amine, were treated with ethylene oxide a similar space would be used but S_x would be different, (Fig. 2-4). It should be evident that Fig. 2-4 and Fig. 2-5 are essentially identical.

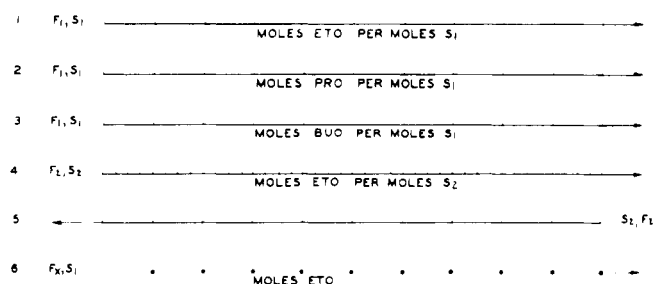


Fig. 2.

Although many of these statements are obvious and trivial at the one-dimensional level, as more dimensions are used they are not as obvious. It should be remembered that the same principles apply to spaces of higher dimensionality. Note that the line segment of Fig. 1 is bounded on each end while the lines of Fig. 2 extend indefinitely in one direction. From each point in such a space as shown in Fig. 2 a new family of materials may be generated by treating the product represented by any point on the line with varying amounts of a different reactive monomer. A new line segment is thus generated from each point on the original line and a plane is defined. Fig. 3 shows how the Pluronic[®]s mentioned above can be represented in such a two-dimensional composition space.

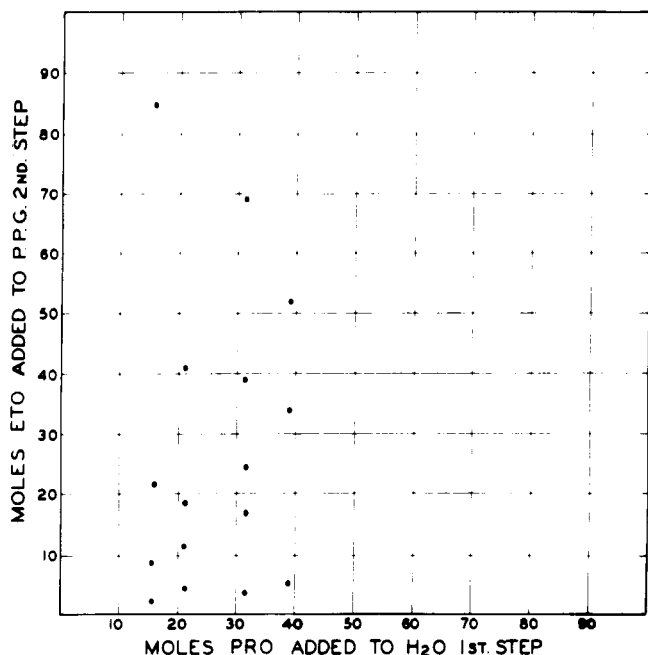


Fig. 3.

Note that this space is non-commutative in that one must first traverse the bottom of the plane until the proper amount of propylene oxide has been reached and then traverse "up" to the proper amount of ethylene oxide. Each point in the space must be reached by such a process and it is forbidden to "back up." This is equivalent to saying that the depolymerization reaction is not the reverse of the polymerization reaction.

A different type of two-dimensional space is shown in Fig. 4. Here the materials to be represented are the Ucons of Carbide and Carbon. These materials are made in a one-step process by treating water with a mixture of propylene oxide and ethylene oxide. The composition of the mixture and the total equivalent moles of mixture added to water may be varied. The bottom of the figure is a line segment of the type shown in Fig. 1. This line is a "selection figure" for the monomer mixture to be used. The vertical dimension represents the number of equivalent moles of mixture added to the starting material. It is the polymerization figure. In this particular space we have delineated certain areas which represent the materials covered by the claims of U. S. Patent 2,754,271 to Kirkpatrick.

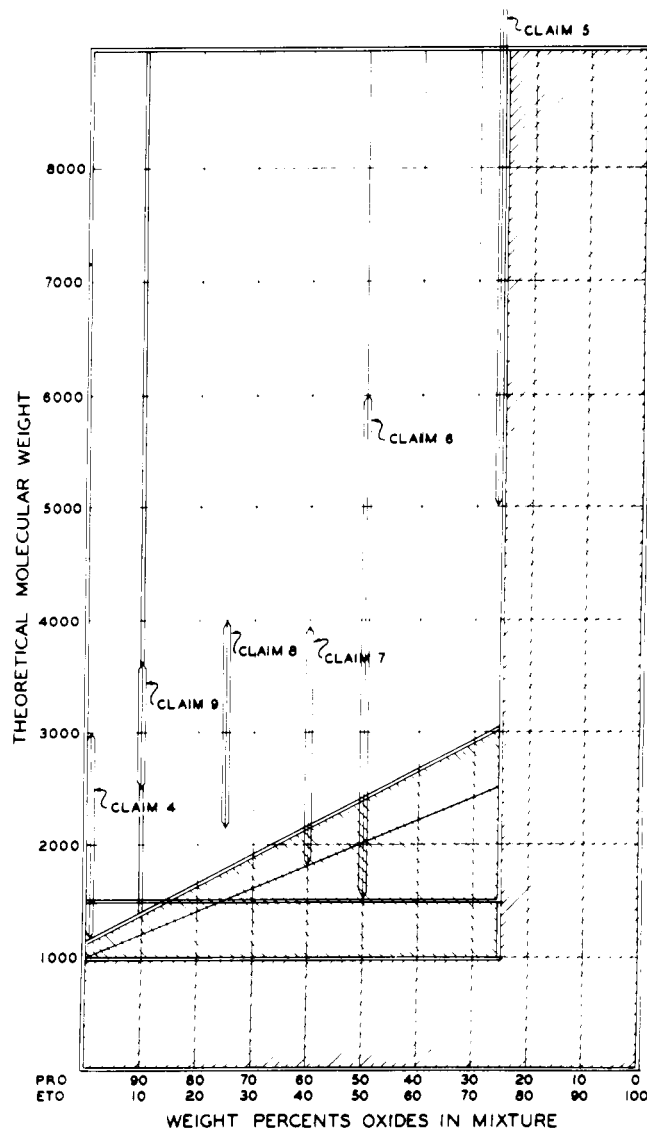


Fig. 4.

One of the useful aspects of this method is the ease with which such information may be displayed and interrelationships between the scope of claims elucidated.

Note that Fig. 3 is bounded on the "bottom" and "left" and extends indefinitely "upward" and to the "right." It represents one quadrant of an unbounded plane. Fig. 4 is bounded on three sides and extends "upward" indefinitely. Such spaces will be referred to hereinafter as "ribbon" spaces.

Fig. 5 is another form of two-dimensional composition space. It serves as a map of all possible compounds that can be made from ethylene oxide, propylene oxide, and butylene oxide by two-step addition of the unmixed oxides. The center of the plane represents one mole of water (or other S_x , F_x). The three dark lines at 120° to each other serve to represent polyethylene glycol, polypropylene glycol, and polybutylene glycol. Each begins with a point selection figure of the specified oxide and is itself a polymerization figure for the pure polyglycol. The six triangular figures into which the plane is divided each represent one of the possible two-stage species of materials that can be obtained by treating a polyglycol with another

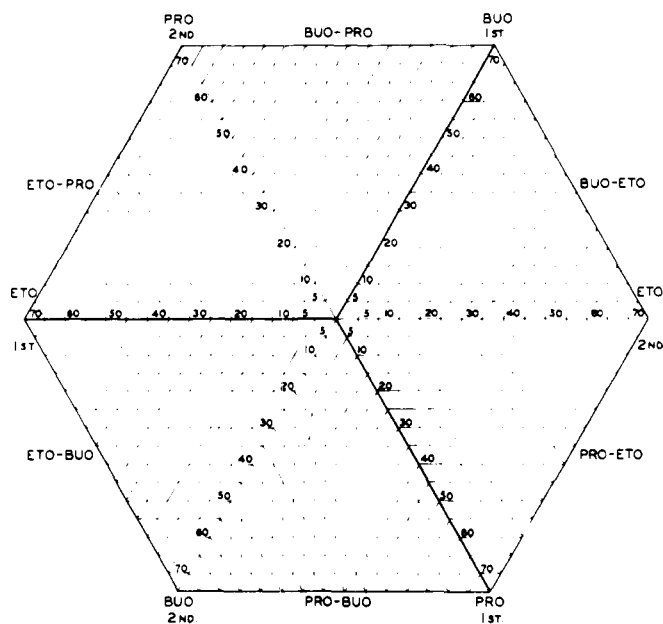


Fig. 5.

oxide. The lower right-hand triangle represents the same materials that are represented in Fig. 3 except that the coordinates are set at an angle of 60° instead of 90° . This example again shows the utility of this method in displaying the relationships between related classes of compounds. Note that this figure is actually six separate figures arranged in a spatial relationship which illustrates the compositional relationships of the classes.

The same principles may be applied to generate composition spaces of three dimensions. Consider the class of materials produced by treating a phenol, stepwise, first with ethylene oxide, then propylene oxide, and then ethylene oxide again. The first-stage materials are easily plotted in a space of the type shown in Fig. 2. The first two stages may be displayed in a space of the type

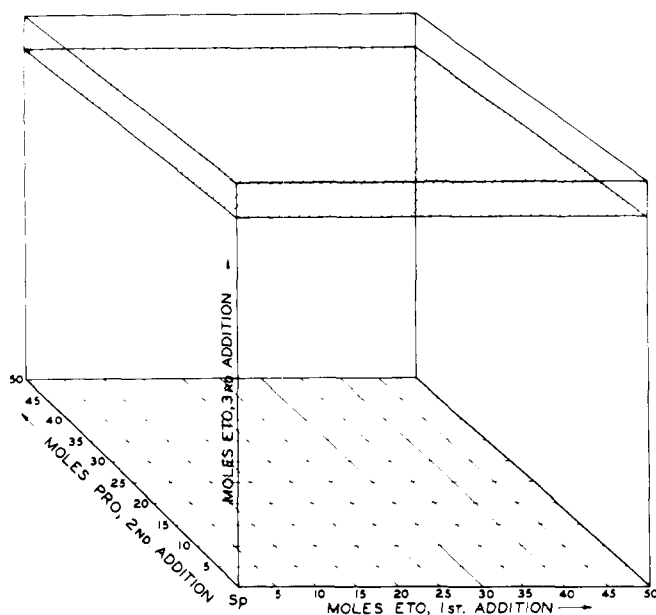


Fig. 6.

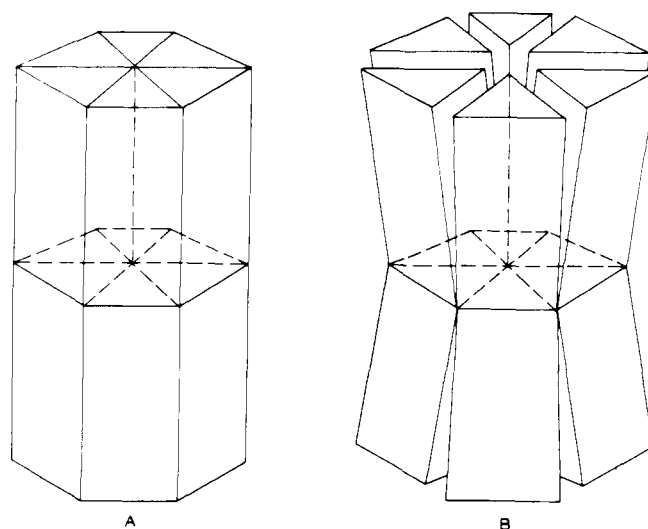


Fig. 7.

shown in Fig. 3. All three stages may be mapped into a "cubic" space of the type sketched in Fig. 6. This is an obvious extension of the technique.

Referring again to Fig. 5, note that each of the six, two-stage classes of materials may be treated with either of the other two oxides to produce a new family of materials. If one of these steps is represented as extending "up" from the plane of Fig. 5 and the other "down," the hexagonal prism of Fig. 7-A is generated. Since, as was noted above, the hexagon is actually composed of six triangles, the prism may be considered to consist of twelve triangular prisms. To keep this relationship distinct, the prisms are caused to diverge slightly as they extend from the generating plane. This is illustrated in Fig. 7-B. If one specifies that a starting material may be treated with either ethylene oxide, propylene oxide, or butylene oxide, stepwise, without mixing oxides, there are three possible one-stage classes, six two-stage classes, and twelve three-stage classes. Fig. 8 shows how these twenty-one classes may be represented in one sort of three-dimensional composition space. This is only one of several equivalent assignments of selection figures that can be made. The method of traverse within this space is analogous to the chemical steps used to synthesize the represented materials. One must start at the center of the base hexagon. Here are specified $S_1 F_1$. At this point a point selection figure requires one to choose one of the three oxides for the first addition step. With the oxide selected, polymerization is represented by traverse along one of the three solid lines. In Fig. 8 if propylene oxide were selected the polymerization figure would extend "down diagonally to the right." When the desired amount of oxide has been added a point is defined. Here a selection of one of the other two oxides must be made. This is equivalent to deciding to go "right or left" from the line. If ethylene oxide is selected the polymerization traverse is into the triangular area labeled PE in Fig. 8. Again when the desired amount of oxide has been added a new point is defined. Again a selection must be made between two oxides and as the selected oxide is added to the two-stage product, the polymerization traverse is "up" or "down." It should be noted that a new F_1 may be specified at each addition stage if desired.

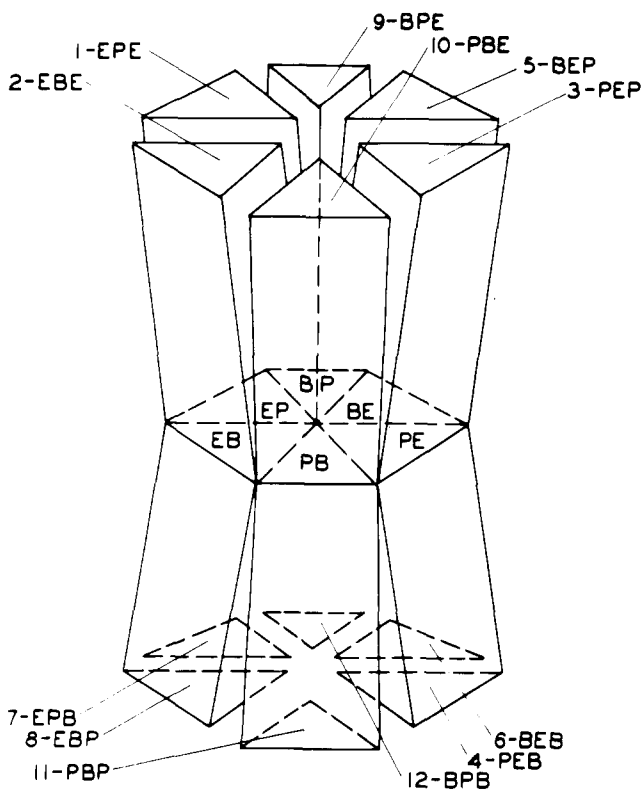


Fig. 8.

As another example, suppose it is wished to display all the possible polyglycols that can be made in a one-step process from ethylene oxide, propylene oxide and butylene oxide using either the single or unmixed oxides or any combination of mixed oxides. All possible monomer combinations can be displayed on a selection figure such as Fig. 9. All possible mixtures of three oxides are provided for in the inner portion of the triangle, all mixtures of two oxides are assigned to the appropriate edge of the triangle, and the three pure oxides are assigned to the corners of the triangle. A prism can now be generated by assigning "equivalent moles of reactive monomer reacted with base material" to the "up" direction. This is illustrated in Fig. 10. The triangular base is a selection figure for the composition of monomer and the prism is the polymerization figure for the one-step process. The same technique may be used to display the reaction products of any other three reactive monomers. The starting material does not have to be water. Similarly, all possible mixtures of four reactive monomers may be displayed in and upon a tetrahedron. Fig. 11 shows how this may be done. The four "corners" represent the pure components, the edges the two-component mixtures, the faces the three-component mixtures and the body of the tetrahedron the four-way mixtures. Notice carefully that this is a selection figure for composition of reactive monomer—not a polymerization figure. Once the monomer composition has been selected from this figure a point in the figure has been defined. A new or "fourth" dimension is then assigned to equivalent moles of monomer reacted with $S_x F_x$. The four-dimensional space thus generated is the polymerization figure for this system. More will be said about polydimensional spaces later.

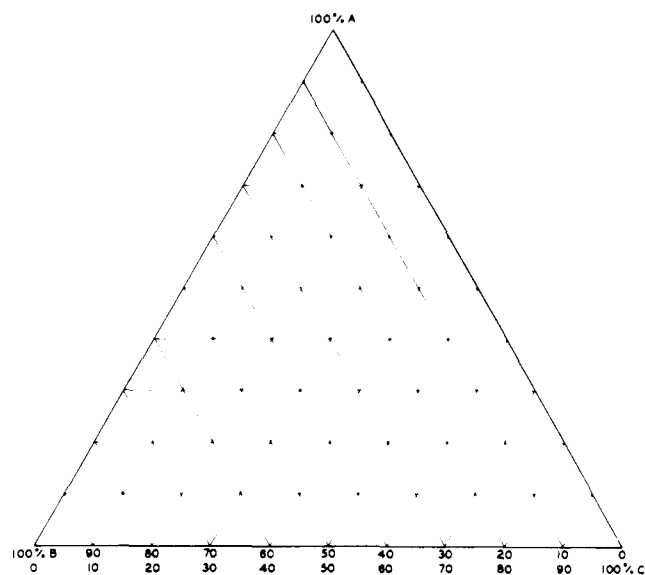


Fig. 9.

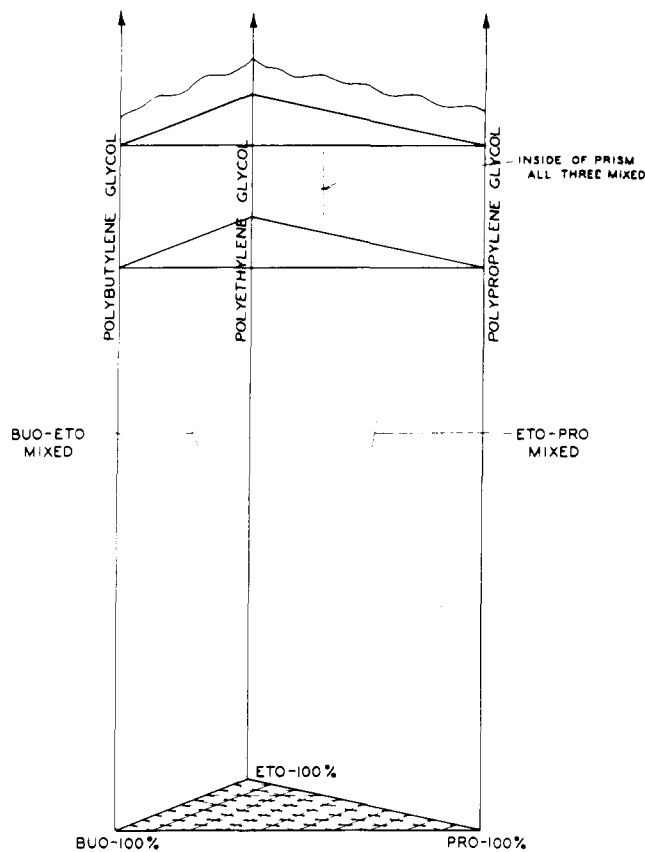


Fig. 10.

Fig. 12 represents another type of three-dimensional space. In this figure the base plane is a ribbon space of the type shown in Fig. 4. Specifically, this ribbon represents the Ucons of U. S. Patent 2,425,845, which are made in a one-step process by treating one mole of water with mixtures of propylene and ethylene oxide. The far left edge of the ribbon represents the polypropylene glycols and the far right edge the polyethylene glycols. If materials represented on this ribbon are further treated

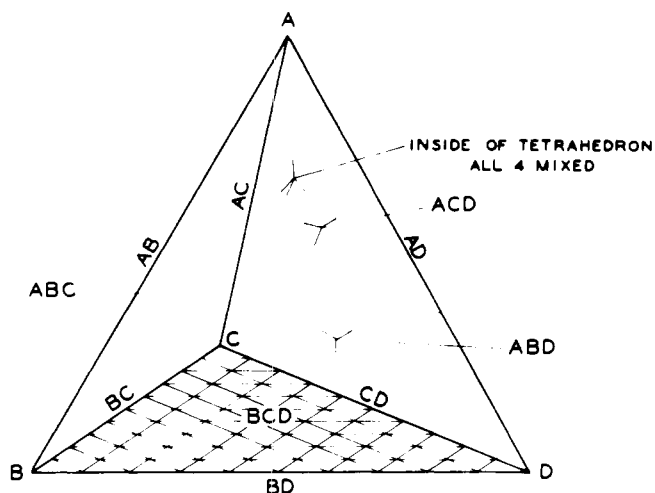


Fig. 11.

with propylene oxide ("up") or ethylene oxide ("down") the materials may be displayed on the "slabs" thus generated.

At this point it should be noted that a given family of materials may be displayed in several different ways. For instance, the Pluronics are displayed on Fig. 3, 5, 8, and 10. The method displaying should be chosen which most conveniently represents the aspects of the problem under study.

It should be clearly understood that the "spaces" of this method bear no relationship to "real" space. Terms such as "up," "down," "right," etc., have been used in discussing "directions." Any resemblance of these terms in composition spaces to their meaning in the three-dimensional space that we feel we live in is purely by way of analogy. In dealing with higher dimensional spaces,

any tendency to associate them with aspects of "real" space is likely to lead to confusion. Multi-dimensional spaces can be used as tools without any concern for "where they are" or "where they go." Because of the conceptual difficulties encountered in dealing with multi-dimensional spaces, we have developed a device whereby such concepts may be more easily displayed. Several poly-dimensional spaces will be discussed in conjunction with a description of the device.

It is difficult enough to represent three dimensions in a two-dimensional sketch; to try to represent more than three dimensions is seldom practical. For that reason this device has been developed. Just as a slide rule embodies a table of logarithms in a simple device, so this device serves as a composition-space analog of remarkable simplicity while possessing great versatility and utility.

The device consists of several rigid transparent sheets bearing grids of various kinds and suitable means of arraying these sheets. I have found it convenient to construct the sheets from clear polymethylmethacrylate and to scribe the grids thereon so that the scribed lines may be filled with a pigment or paint to make the lines of the grids more visible. Three different kinds of grids are usually employed, as illustrated in Fig. 13, a rectangular grid, a triangular grid, and a "ribbon" grid. Other grids may be employed as needed.

As an example of how this device is employed reference is made again to Fig. 12. Suppose a study is being made of the cloud point of the materials displayed in Fig. 12. Plane ABCD is represented by a sheet bearing a "ribbon" grid. Other sheets bearing rectangular grids are arrayed, by any suitable clamping means, at right angles to the ribbon sheet to represent such planes as EGHF, BCVT or JNQK. As the cloud points of specific members of the group of materials are determined they are written

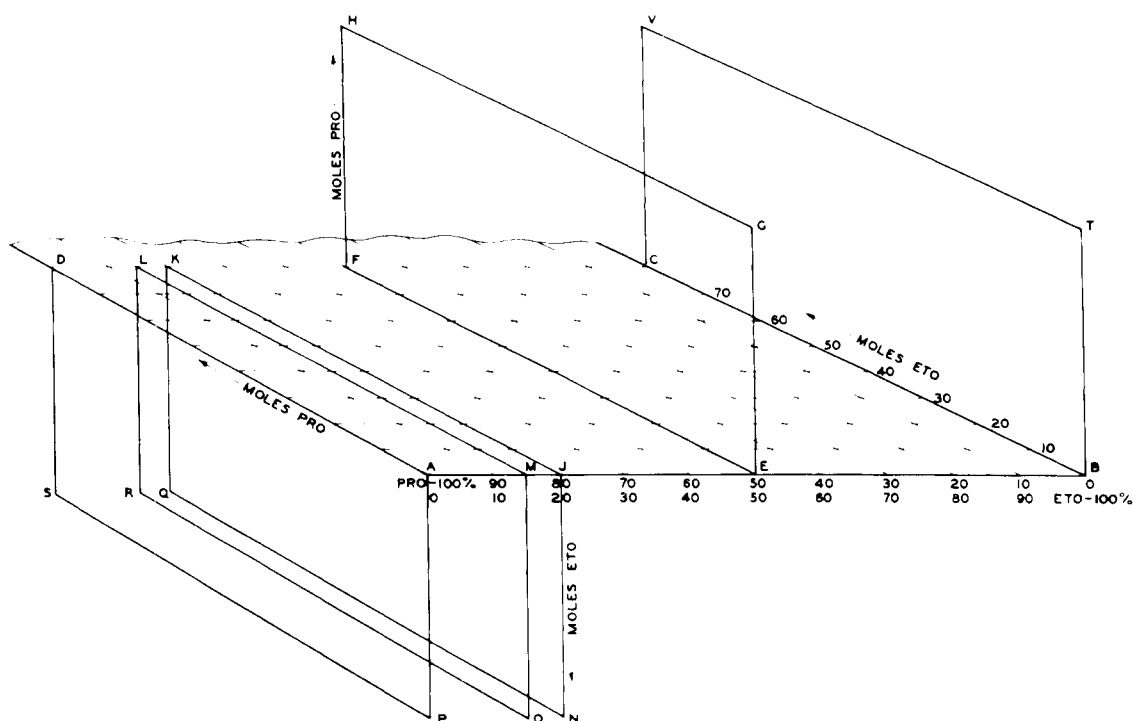


Fig. 12.

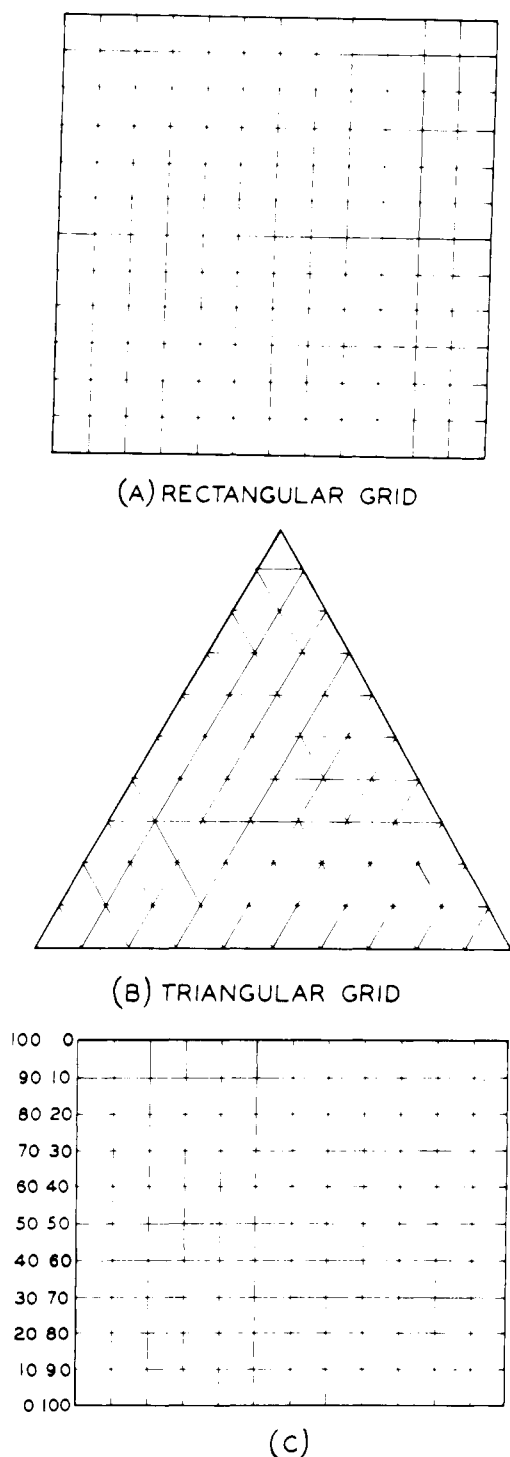


Fig. 13.

with wax pencil or other suitable means upon the appropriate sheet at the point which represents the composition of the specific material. When all the data have been transferred to the composition space, relationships which would be extremely difficult to detect from the tabular data can readily be seen. For instance, lines may be drawn between points of equal cloud point and so "iso-cloud point" lines, surfaces and volumes delineated. In fact any determinable property may be displayed on such a device and several properties simultaneously displayed by the use of different symbols or colors so that the

variation of several properties with respect to composition may be studied at the same time. Optimal regions in the composition space for any property may thus be discovered and by determining where optimal regions for different properties overlap it is possible to determine the optimum composition for a combination of properties. Since the number of individual materials which may be prepared in a group such as this is virtually infinite, it is necessary from a practical standpoint to prepare as few members of the class as possible and from them determine the specific members which have utility for a particular purpose. The use of this device makes the choice of individual compositions to be prepared much easier. The usual procedure is to prepare a small number of examples of the class, determine whatever properties of these members are pertinent to the problem at hand, and display these properties on the device. It is then usually possible to find "composition directions" which tend to maximize the properties. New materials can then be prepared which are located within the regions of the composition space where the properties maximize. These are then added to the display. The method thus greatly reduces the number of materials that must be prepared in an investigation.

This device is particularly useful in dealing with multi-dimensional composition spaces. Suppose, for example, that a group of polyglycols is made by starting with water and adding, stepwise, first ethylene oxide, then propylene oxide, then ethylene oxide again, then butylene oxide, then ethylene oxide again. This is five stages of addition and requires a five-dimensional composition space to display the materials in a formal, mathematically rigorous manner. However, the first three stages can be displayed easily on the device by arraying several rectangular grids, one above the other, to form a space of the type illustrated in Fig. 6. The three-stage products can then be sorted into sub-classes, each class having the same amount of ethylene oxide added in the third step. Each of these classes will fall on a plane in the composition space represented by a grid in the device. If each of these planes is made the base of a new cubic space, the fourth step may be displayed. In the same manner planes may be selected in these spaces and the fifth step displayed in a new set of cubic spaces. Alternatively, a "line" may be selected in the three-stage cube and this line made the base line for a new cubic space which can be used to display the fourth and fifth steps.

As the complexity of the system under consideration increases, the utility of the method becomes even greater. The ease with which complex systems may be represented and the clarity with which they may be displayed makes it possible to discover relationships between composition and function which could be detected only with great difficulty by other methods.

An example of the power of this method is given in Fig. 15, 16, and 17. These three figures display data cited in a patent application.

In this instance 261 specific examples of compositions are cited. This takes 12 typewritten pages just to cite the compositions of the examples. The solubilities of these examples are also cited. This takes 31 more typewritten pages. All of these data are displayed in Fig. 15, 16, and 17. In addition, data on the base materials are contained in

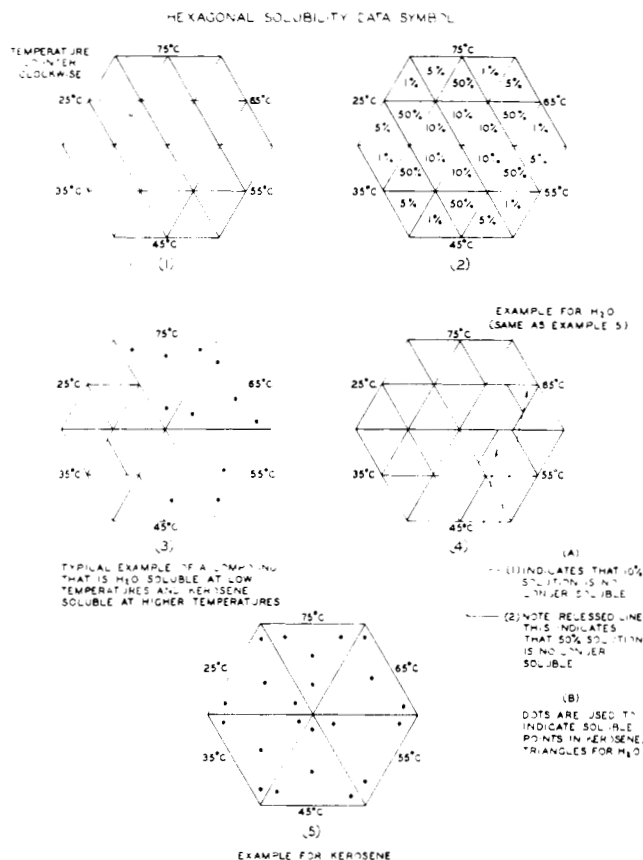


Fig. 14.

Fig. 15. These three figures contain nearly 15,000 separate pieces of data, each of which can be read directly from the display. The three figures were developed in the following manner. The device was arrayed to conform to a composition space of the type shown in Fig. 12. Fig. 15 corresponds to the plane EFGH of Fig. 12, Fig. 16 corresponds to the plane JKQN, and Fig. 17 corresponds to the plane MLRO.

Solubility was determined in distilled water and in kerosene at concentrations of 1%, 5%, 10% and 50% by volume.

For each individual composition the solubility tests yield 48 separate datum, all of these data may be displayed by the use of an appropriate symbol system. One way this may be done is illustrated in Fig. 14. The symbol is based on six equilateral triangles grouped into a hexagon. Each triangle represents one temperature at which solubility was determined. Starting from the upper left-hand triangle of the hexagon and proceeding counter-clockwise, the triangles represent the solubilities at 25°, 35°, 45°, 55°, 65°, and 75°. Each triangle is further subdivided into four smaller triangles. Each of these four triangles represents a different concentration of the material under test, specifically, 1%, 5%, 10%, and 50%. If the material under test is soluble in water at the specified concentration, the concentration triangle is drawn in. If not it is omitted. If the material is soluble in kerosene, a dot is placed in the center of the appropriate concentration triangle. In this manner, an unambiguous symbol can be generated for each possible solubility profile. These

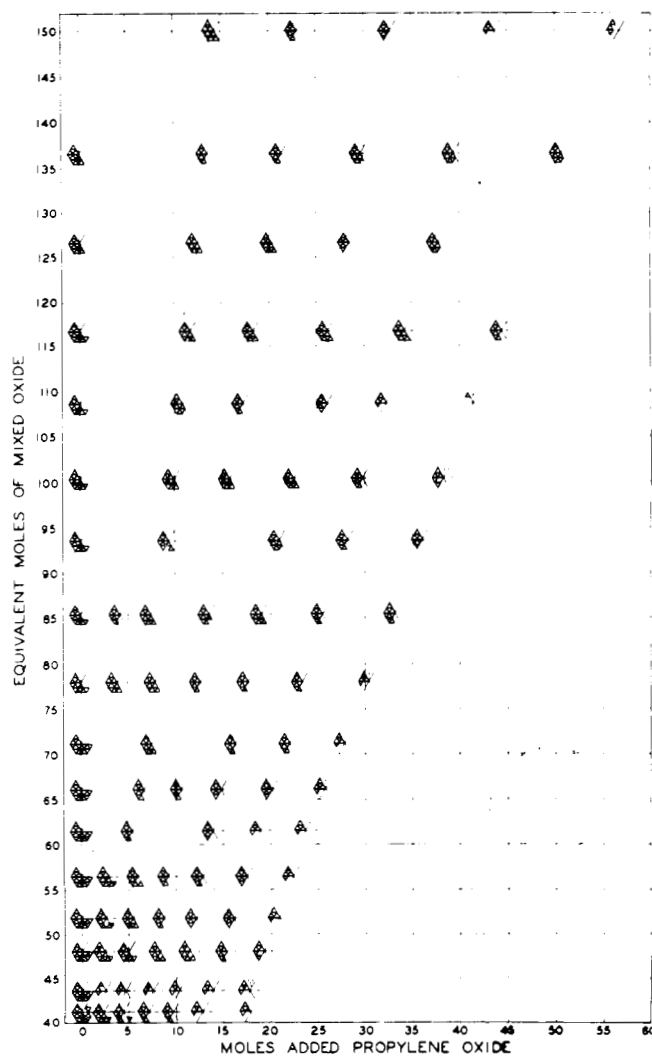


Fig. 15.

symbols can then be mapped onto the proper composition space representation.

Figures 15, 16, and 17 were generated by placing the appropriate solubility symbol for each example at the point in the figure that corresponds to its composition in the composition space. Thus it is possible to condense 43 pages of tables into three figures. Furthermore, by arraying the figures in the proper spatial relationship to each other an example of the type of device discussed here is obtained which makes it possible to examine the variation of solubility with composition. "Regions" of water solubility can be easily mapped and transition zones delineated. Examples of related composition are displayed in proximity to each other and thus may be easily compared. Comparable evaluation of the data directly from the tables is almost impossible.

Consider further the general class of polymers which may be represented by a multi-step system where each polymerization step is preceded by a selection figure of the type shown in Fig. 11. Simple calculation will show that there are 15 sub-classes for one stage of polymerization and, in general, 15^n sub-classes for n stages of polymerization. This means that a five-stage polymer can belong to one of at least 750,000 sub-classes. While nothing

is to be gained by listing these sub-classes in detail, it should be pointed out that this method makes it entirely practical and possible to do so. Furthermore, any specific polymer can be easily assigned to its proper sub-class and its relationship to other classes easily displayed.

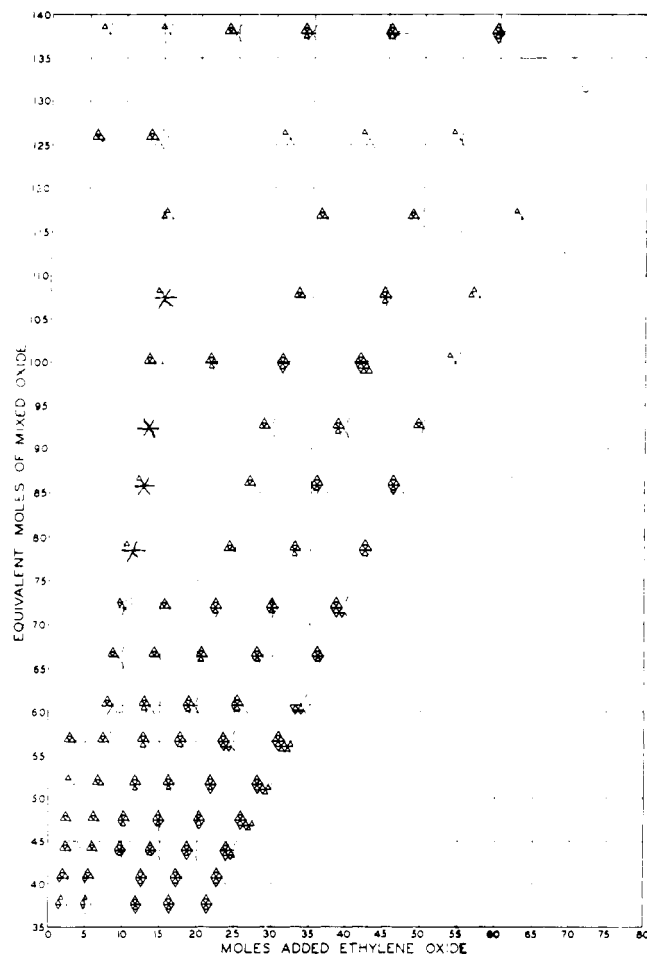


Fig. 16.

As a specific example, I will consider the system where, in the selection figure of Fig. 11, A is ethylene oxide, B is 1,2-butylene oxide, C is propylene oxide, and D is propylene sulfide.

Table I lists a group of polymeric materials which fall

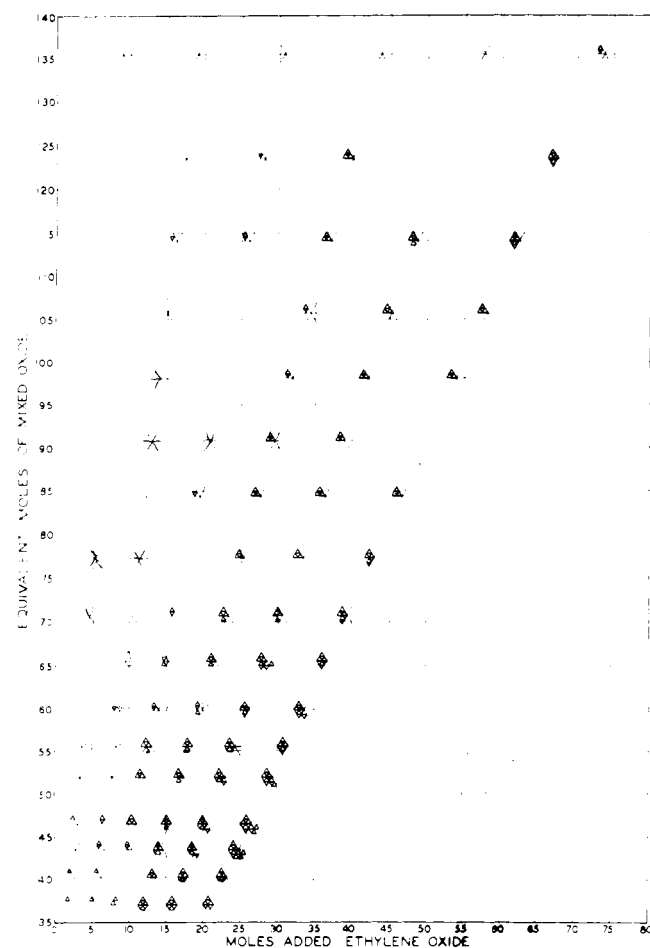


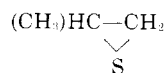
Fig. 17.

Table I

Ex.	Step I		Step II		Step III		Step IV	
	Monomer composition	Moles ^a added	Monomer composition	Moles ^a added	Monomer composition	Moles ^a added	Monomer composition	Moles ^a added
1	EtO/BuO	32.2						
2	{ 7/3 w/w	32.2	PrO 100%	10				
3	EtO/BuO	32.2	PrO 100%	10	EtO 100%	15		
4	{ 7/3 w/w	32.2	PrO 100%	10	EtO 100%	15	PrS ^b 100%	5
5	PrO 100%	2	EtO(PrO)BuO	13.4				
6	PrO 100%	2	{ 6/2/2 w/w/w	13.4	PrS ^b 100%	3		
7	PrO 100%	2		13.4	PrS ^b 100%	3	EtO 100%	10
8	PrO/PrS	8	EtO 100%	14				
9	{ 1/1 w/w	8	EtO 100%	14	PrO/BuO			
		8			2/1 w/w	5		
10	PrO 100%	2	PrO/BuO	35				
11	PrO 100%	2	{ 3/7 w/w	35	EtO 100%	30		
12	PrO 100%	2		35	EtO 100%	30	PrS ^b 100%	12

^a Moles based on oxirane equivalents.

^b PrS means propylene sulfide



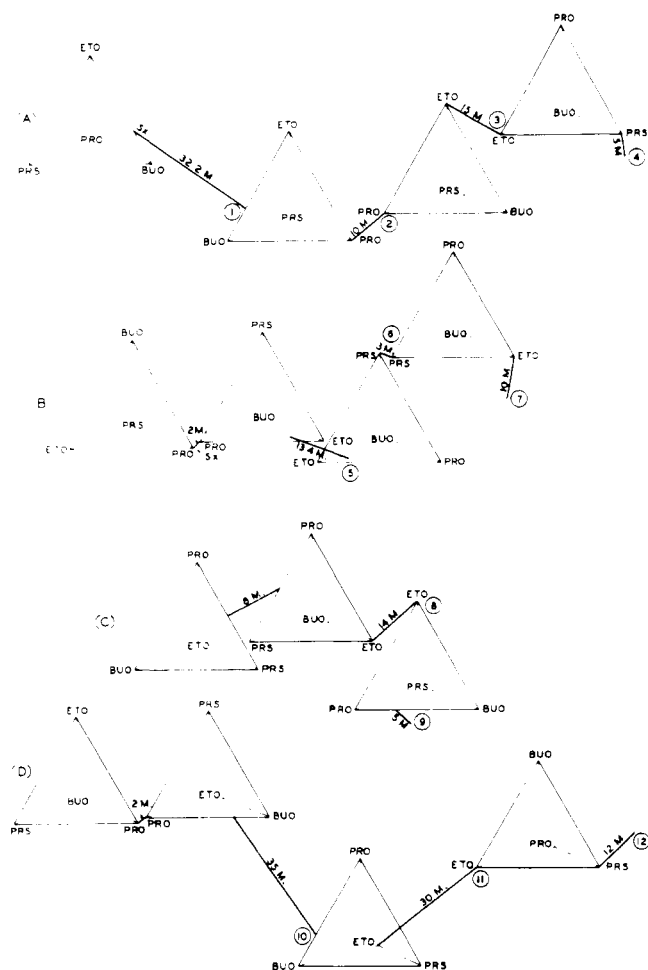


Fig. 18.

in this system. For simplicity S_x in this case is taken as water and only the first four polymerization stages are considered.

Fig. 18 shows how this method may be used to show the interrelationships between individual members of related sub-classes. Fig. 18-A begins with a selection figure wherein the $\frac{1}{3}$, w/w ratio of mixed ethylene oxide-butylen oxide is selected and then 32.2 equivalent moles

of this mixture are allowed to react with one mole of water to produce Example 1 of Table I. The next selection tetrahedron in the chain shows the selection of unmixed propylene oxide as the next reactant. Ten moles of this are added to one mole of Example 1 to obtain Example 2. The next selection tetrahedron shows the selection of unmixed ethylene oxide as the next reactant. Fifteen moles of this are reacted with one mole of Example 2 to obtain Example 3. The last selection tetrahedron in the chain shows the selection of unmixed propylene sulfide as the final reactant. Five moles of this are treated with one mole of Example 3 to obtain Example 4. In a similar manner Fig. 18-B shows the relationships between Examples 5, 6 and 7 of Table I; Fig. 18-C shows the derivation of Examples 8 and 9; and Fig. 18-D shows the derivation of Examples 10, 11, and 12.

It can easily be seen that this method makes it possible to select and depict unambiguously the fifteen specific sub-classes involved in the examples of Table I from the several thousand possible sub-classes without a laborious tabulation of all possible classes. It should also be noted that many variations of the recited examples are made immediately apparent by study of Fig. 18. This predictive capacity of the method is one of its most useful aspects.

In the Examples of Table I and Fig. 18 each selection figure involves the same four reactive monomers. It is entirely possible to change both the type of selection figure and the combinations of reactive monomers depicted in the selection figures in constructing an array to depict a particular series of polymers. The selection figure type and the assignment of reactive monomers to a selection figure may be varied as desired for purposes of clarity, brevity, or to emphasize specific interrelationships.

A further advantage of this approach to the over-all problem is that the appropriate composition space for a given problem provides an organized matrix for filing data. A punched card or other data filing system can be indexed according to the coordinates of the composition space and thus provide ready filing and retrieval. With such a system each individual polymer has a unique "name" in a sequential notation and all data pertaining to that polymer can be filed under that index entry. Searches can be run for specific polymers, sub-classes of polymers, or polymers with specific properties.