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# Future of Petrochemical Raw Materials in Oleochemical Markets

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ABSTRACT

The petrochemical industry (PCI) has undergone profound changes during the last decade and is continuing to adjust to changing world economic conditions. One of the most important of these is the price of crude oil. Although an equilibrated pricing structure remains to be demonstrated, anticipated adequacy of supply and versatile, innovative methods of converting crude and natural gas to high valued products assures it a vital and healthy future. The product areas in which the PCI and the oleochemical industry (OCI) overlap are actually quite small in terms of the total capacity. In those limited areas of overlap, we expect the role of the PCI during the next several years to continue to be one of a complementary nature. By providing security of supply at competitive prices, it will create confidence and reliability which will benefit both the petrochemical and oleochemical industries. And most significantly, the resources of the petrochemical industry will also allow it to respond to new market conditions, particularly those of accelerated volume needs and specific performance, with the flexibility and creativity which have been its hallmarks.

#### INTRODUCTION

Markets supplied by the petrochemical and oleochemical industries are, for the most part, quite different. Yet, over the years, several important areas of overlap have evolved. Generally, this has occurred as a result of penetration of existing oleochemical markets by new synthetic materials.

There are four general product groups which account for most of this overlap: glycerin, short-chain linear fatty acids, fatty alcohols and fatty amines. Total world production of these four product groups is ca. 1.5 million metric tons, excluding production of Eastern Block nations. The relationship of this overlap volume is put in perspective in Figure 1. It shows that this total volume represents ca. 25-35% of the oleochemical industry, depending on the estimate one uses for its size. By comparison, that volume represents slightly over 1% of the petrochemical industry (PCI).

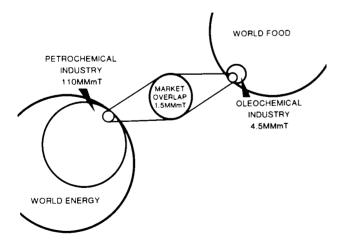


FIG. 1. Petrochemical-oleochemical overlap.

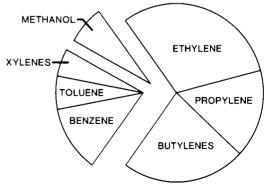
driven by much bigger "flywheels": world energy and food dynamics, respectively. Whereas the intercompetitive strengths of the PCI and OCI depend heavily on relative feedstock costs as determined by these flywheels, efficient and innovative use of feedstocks allows considerable control over ultimate product costs. With this thought, we will look at trends within the PCI over the last decade and discuss how the industry has managed to cope with some dramatic changes. In this way, we hope to be able to understand better the future impact of PCI raw materials on selected oleochemical markets.

#### PETROCHEMICAL INDUSTRY OVERVIEW

Let us first consider the PCI itself. It is a worldwide business and any discussion of the industry must be global in nature. Although many examples in this paper are based on situations from the United States and Shell Chemical Company specifically, the conclusions we draw, we believe, are illustrative of the industry in a broader sense. The time frame for this discussion will be the 30-year period between 1962 and 1992. This covers the period of rapid growth of petrochemicals in the 1960s, the two "oil shocks" in the 1970s, and allows a 10-year look into the future.

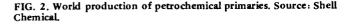
For quantification of the PCI, I will refer to the production and utilization of olefins, aromatics and methanol. Figure 2 shows world production of these products in 1979. World production in this case and others to follow will exclude that of Eastern Block countries. The olefins category includes ethylene, propylene and butylenes. Aromatics include benzene, toluene and xylene. The rationale for defining quantities in this way is that it conveys the concept of these materials as basic "building blocks" for all petrochemical derivatives. It also avoids accounting for intermediates which are eventually converted to end-use products. Using this approach, total volume is somewhat understated because inorganics, particularly nitrogen, chlorine, sulfur and oxygen, are incorporated into the final products in many cases.

Data for this paper come from both Shell Chemical Company and from outside sources including the US Government and consultant firms closely involved with the industry. Crude oil price projections will be from non-Shell sources.



1979 TOTAL: 110 MILLION METRIC TONS

In Figure 1, the PCI is shown in terms of its supply base -energy-and the oleochemical industry (OCI) in terms of its supply-food in the form of fats and oils. Both the petrochemical and the oleochemical industries are thus



In a historical sense, the petrochemical industry really began during World War I, when the first commercial petrochemicals, isopropyl alcohol and acetone, became available in the USA from Standard Oil of New Jersey. Within 65 years, the PCI has grown into a 100 million metric tons per year industry. In 1979, 44% of the world's petrochemical capacity was located in North America, 35% in Western Europe, 17% in East Asia and 4% elsewhere.

As the PCI has grown, it has undergone massive technological change. In the beginning, basic petrochemicals were isolated from crude oil refinery streams by simple smallscale distillation. Relatively simple chemistry was used to convert these primaries into first-order derivatives such as acetone and methyl ethyl ketone. World War II prompted the development of larger scale units for production of strategic materials such as synthetic rubber based on butadiene. Natural gas liquids, particularly ethane and propane, became widely available in the 1940s and new thermal cracking technology was developed to use these materials.

By the 1950s, the PCI was positioned for substantial growth. High quality end-use products were developed and significant penetration began into markets for traditional materials such as wood, metal, paper and glass. The feedstock base was expanded during the 1960s by the use of catalytic cracking and hydrotreating to increase gasoline production. The partnership between the petrochemical and petroleum refining industries was further strengthened by the advent of large-scale thermal cracking of heavy crude oil fractions to yield "on-purpose" light olefins and aromatics. By the early 1970s olefin plants with capacities in the 500,000 metric ton range were in operation. During this period, derivative manufacturing plants also began to grow in size. This tendency toward efficiency through scale has continued up to the present. For example, new polyethylene plants can easily be 250,000 metric tons in size.

The PCI is, therefore, characterized by bigness. But scale alone has not been the major achievement. Innovative and integrated technology has driven the PCI throughout its development. Timely application of advances in synthetic organic chemistry and new engineering techniques have contributed to its creativity and flexibility. Figure 3, despite its complexity, is a very simplified schematic of the technologically based network of processes which make up the petrochemical industry. It shows how primary olefins and aromatics are processed into intermediates and then into end-use consumer products. One such sequence for the production of polyvinyl chloride (PVC) is shown by the shading in Figure 3. PVC is, of course, fabricated into a large number of consumer items such as leather cloth for automobile upholstery.

Another example of a large-scale technically integrated process is the ethylene-based manufacture of detergent alcohol products. Shell Chemical Company makes these products at facilities located in Geismar, Louisiana, using a specific proprietary technology. The process is known as the Shell higher olefins process (SHOP). SHOP was developed in the early 1970s and streamed in 1977. It is based on oligomerization of ethylene into a full range of  $\alpha$ -olefins as shown in Figure 4. Some of the  $\alpha$ -olefins are distilled and sold directly into a variety of markets. Some are converted into internal olefins in a second phase of SHOP. Internal

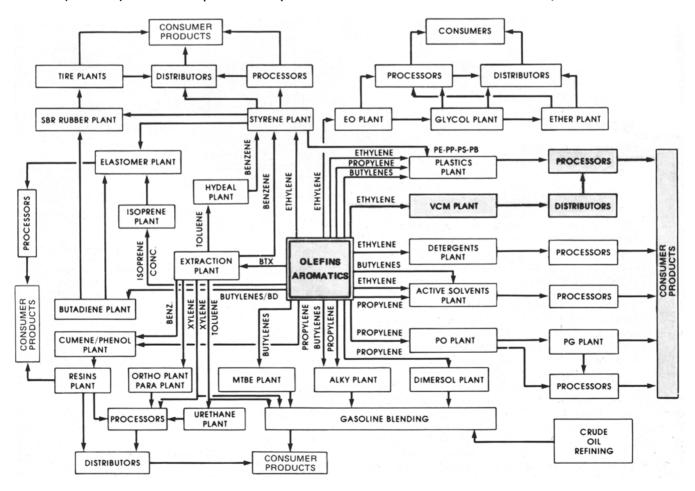


FIG. 3. Petrochemical industry network.

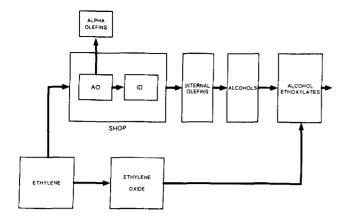


FIG. 4. Shell Geismar petrochemical network.

olefins in the detergent range are then converted into alcohols with Shell's hydroformylation process. These alcohols can be sold directly or processed further, with ethylene oxide, into alcohol ethoxylates. These ethoxylates are used directly in many consumer detergent products. The total facility for these operations consumes over 400,000 metric tons of ethylene annually. It is integrated with captive ethylene and ethylene oxide, and it is versatile, producing a wide range of olefins, alcohols and surfactants. This combination of size, integration and advanced technology is characteristic of today's petrochemical industry.

#### PETROCHEMICAL INDUSTRY TRENDS

With this abbreviated background on the PCI, let us now consider some of the trends which affect it.

The most important trends to examine are feedstock costs, volume growth, geographical production shifts and technology changes. As everyone knows, the world has undergone two crude oil price shocks within the last 10 years. Dramatic increases took place in the 1973-74 and the 1979-80 time frames. As the price of crude oil increased, so did the cost of petrochemical feedstocks. Ethylene, benzene and crude oil prices during this period are shown in Figure 5. In the USA, natural gas has been controlled at artificially low prices and this advantage helped expand US petrochemical exports for a while. But this advantage is disappearing as gas gradually moves toward an equivalency on an energy content with crude oil. The price of crude oil will, for this reason, in the foreseeable future, play an important role in setting prices for petrochemicals.

Projecting the price for crude oil over the next 10 years would be difficult at best. In the third quarter of 1983, the contract price of crude is ca. \$29/barrel, but there are numerous scenarios predicting higher and lower prices. If we look back at long-range price projections made just 3 years ago, we can see how far off those guesses were compared to the actual price today.

In late 1979 and early 1980 during the second oil shock, projections for crude oil in 1990 tended to be in the upper range of the shaded area of Figure 6, i.e., upwards of \$70 per barrel. By the end of 1982, with demand reduced by economic recession, much lower prices were being predicted, some even below those of 1983. The important point is that the PCI has been able to absorb the oil price shocks of the 1970s and remains a vital, important part of the economy. Whatever crude oil prices are in the 1980s, probably in the lower range shown, we believe the PCI will continue to respond and remain viable. We have several reasons for saying this and I will now describe them.

Without doubt, the oil increases caused a slowing of petrochemical growth. The US production of ethylene between 1960 and 1982, as shown in Figure 7, illustrates this point. A prolonged world recession which slowed overall economic growth, together with those dramatic step changes in petroleum prices, brought about, in the opinion

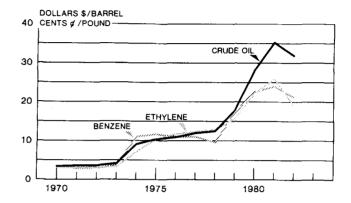


FIG. 5. US prices for ethylene, benzene and refiner acquisition cost for crude oil, 1970-82, current dollars. Source: US Department of Energy, US International Trade Commission, SRI.

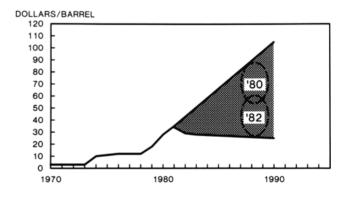


FIG. 6. Crude oil price projections, 1980 vs 1982. US refiner average acquisition costs, current dollars.

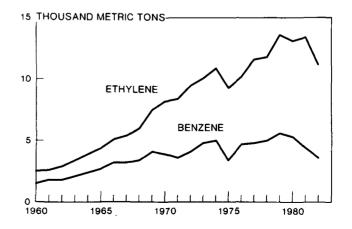


FIG. 7. US production of ethylene and benzene, 1960-82. Source: US International Trade Commission, SRI.

of many observers, an early maturity to the industry. Producers began to shut down their oldest and least efficient units. For example, in 1982, world ethylene capacity as well as production was less than in 1981. This is the first time such a decline in capacity has occurred (1).

A gradual shift of production capability for basic chemicals is occurring from industrialized nations to "feedstock rich" countries. In areas such as the Middle East, natural gas has been flared in the past because there have not been adequate collection facilities or local markets. This situation is also changing. Several companies, for example, are now constructing large petrochemical complexes in joint ventures with the Arabian government. If all of these are streamed as planned, they will represent ca. 5 million metric tons of capacity by 1986. In other areas of the world, such as Mexico and Canada, chemical development is being encouraged by government policies aimed at upgrading crude oil and natural gas. In Mexico, for example, a goal of the government is to have over 30 million metric tons of petrochemical capacity in place by 1990 (2).

In Canada, the government has taken a major role in pricing natural gas so that it will be able to compete as a feedstock for the developing petrochemical industry.

By 1990, 10-15% of the world's petrochemical capacity will be located outside the traditional areas of North America, Western Europe and East Asia. This is up from less than 5% in 1979. Much of this capacity is being built for export, since producing locations will not be able to consume all the output. Although the new plants still represent a very modest part of total capacity, they will have state-of-the-art technology and will be based on relatively inexpensive feedstock. Additional less efficient units throughout the world will most likely shut down, leading to greater competitiveness of the PCI overall.

In the recent past, increasing feedstock prices have put a strain on petrochemical margins. According to the US Department of Commerce, the cost of materials for all petrochemicals in the USA increased from 48% of selling price in 1972 to 65% in 1980, for a 37% increase. This effect has been especially significant in the plastics area. For example, a recent Shell Chemical study (3) showed that during this time, costs for raw materials for major thermoplastics in the USA increased from an average of ca. 30% to over 60% of selling price. Such increases put a new emphasis on cost controls for feedstock and process energy. The PCI has responded with a burst of technology improvements which have led to such things as more effective catalysts, better feedstock versatility, and lower energy and capital intensive processes.

The manufacture of ethylene oxide is a prime example of this kind of technology improvement. Three new generations of catalyst with improved selectivity for this conversion have been offered since the 1960s. As a result, the ethylene raw material is used much more effectively.

In the feedstock area, an example of improvement lies in the fact that most ethylene producers have modified their plants to allow flexibility in feedstock choice. Some plants can process feeds which range from ethane up through naphtha and gas oil. Figure 8 illustrates some of the potential feeds which can be used to produce ethylene and the associated coproduct slates. This versatility allows olefin producers to optimize their operations as a function of feedstock prices and coproduct values.

Another example of PCI technology in action is linear low density polyethylene (LLDPE). Polyethylene has been manufactured for decades and must be regarded as a mature product. But, new technology introduced within the last 5 years has created a revolution in the industry. Union Carbide, Dow and other companies have introduced new

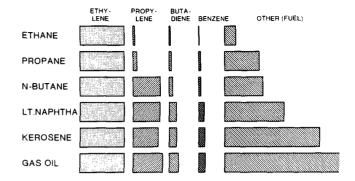


FIG. 8. Olefin plant product yields. Source: Shell Chemical,

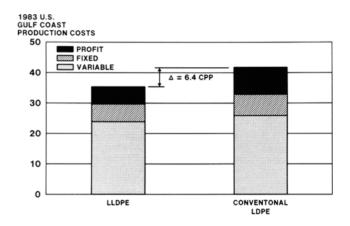


FIG. 9. Polyethylene production costs. Conventional low density vs linear low density, cents per pound (CPP). Source: Chem Data Inc.

energy- and capital-saving processes for its manufacture. Polyethylene is superior in performance to the established product. For example, LLDPE can be fabricated into plastic film using 20% less material than conventional polyethylene. The cost savings associated with this new technology are displayed in Figure 9. In this example, all segments of the cost structure are less expensive for LLDPE than conventional polyethylene. The total difference in cost is ca.  $6.5 \pm$ /lb. This is significant in the very competitive polyethylene business.

The technology changes which I have mentioned are some of the results of a very active research and development program which is characteristic of the PCI. In 1981, ca. 15% of all US industry R&D was funded by the "chemicals and allied products industry," of which the PCI, of course, is a part. This is remarkable, since this industry accounts for less than 2% of the US gross national product (4). R&D for the US chemical industry was up 14% in 1982 vs 1981, and planned spending for 1983 is expected to grow 12% over 1982 (5). Despite severe profitability pressure over the last few years, R&D spending in Europe has also managed to keep pace with or exceed inflation. Several European chemical companies have stated a need for even more R&D, despite stagnation in their profit growth (6). With this kind of attention to R&D, new technology will continue to produce innovation within this industry.

To summarize the recent trends which have characterized the PCI, I would underscore the fact that it has undergone an upheaval within the last 10 years, but it is emerging viable and strong from this time of change. It is responding to unprecedented feedstock cost increases and curtailed growth with shutdowns of inefficient units, with capacity shifts to lower cost feedstock areas, and with continued high R&D effort.

Now, let us look to the future. In considering the future of petrochemical raw materials, it is useful to think of both the continuity and the versatility of supply. By continuity of supply, we mean availability when needed at reasonable and predictable prices. Few forecasters saw the energy increases of the last 10 years. But it should be kept in mind that this period was one of high inflation on all fronts. Petrochemical prices on a constant dollar basis have fared reasonably well, especially after the last oil shock as shown in Figure 10. The major reasons for this have already been pointed out. And, in spite of the rapid price increases and crude oil disruptions, no major discontinuities have occurred in the supply of basic petrochemicals around the world. It is also worth noting that a period of price correction on crude oil seems to be taking place and oil is abundant to the point that one frequently hears the term "oil glut.'

We believe the continuity of petrochemical raw materials will be sustained into the future. Anticipated discoveries of crude oil and natural gas combined with better use of available feedstock will all contribute toward a steady supply. At the beginning of 1983, the world had proven reserves of 670 billion barrels of crude oil and 3 trillion cu ft of natural gas (7). Oil shale and tar sands contain the equivalent of an additional 3.3 trillion barrels of crude oil, and recoverable world coal reserves amount to 615 billion metric tons (8). Obviously, appropriate economic conditions must exist for petrochemical producers to access these sources. But the feedstock is certainly available in very large quantities. In perspective, the world's annual production of petrochemicals uses the equivalent of only 0.1% of the world's proven crude oil reserves.

The second important aspect of the future for petrochemical raw materials is versatility of supply. By versatility of supply, we mean the potential manipulation of raw materials to produce a given product. The very simple building block nature of petrochemicals lends itself well to construction of specific complex molecules. And to a large degree the building blocks are interchangeable depending on price: ethylene can be substituted for propylene, which in turn can be substituted for butylene. Heavy R&D spending will ensure that full advantage is taken of this versatility in developing more complex and more specialized products. Another result emerging from R&D is the extension of the petrochemical building block concept to synfuels technology. Commercial production of chemicals from coal-derived syngas is now taking place. The extent and speed of this development will depend heavily on crude oil economics.

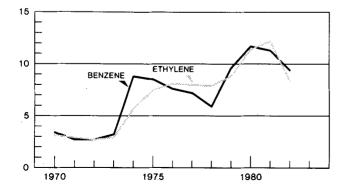


FIG. 10. US prices for ethylene and benzene, 1970-82. 1970 constant dollars, cents per pound. Source: Shell Chemical, SRI.

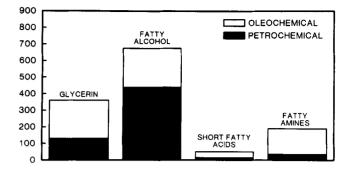


FIG. 11. World production, 1980 (thousand metric tons).

#### IMPACT OF PCI TRENDS ON OCI MARKETS

Let us turn now to specific areas of PCI and OCI overlap mentioned earlier: glycerin, detergent-range alcohols, shortchain linear fatty acids and fatty amines. Glycerin was the first of these to be penetrated by petrochemicals; however, world production is still based chiefly on oleochemical feedstocks. About two-thirds of world production, for example, was from natural feeds in 1980 as shown in Figure 11. This share has increased somewhat in recent years as a result of increased synthetic feed prices, but particularly in the case of glycerin, the whole story is more complex than just feedstock prices (propylene is, of course, the principal raw material for synthetic glycerin). Natural glycerin, on the other hand, is produced by splitting a wide range of triglycerides and to a large extent is free of coproduct dependency on any single fatty acid. Moreover, although glycerin enjoys certain unique end uses, there are significant demands where substitution can occur on a cost performance basis. Other well known materials which can be used in these substitution situations are sorbitol, propylene glycol, pentaerythritol and butanediol. The last three are made by petrochemical processes. So within the total spectrum of potential glycerin applications, the flexibility offered by the PCI building block approach is still important. It allows users to match products having various physical and chemical properties to specific needs. This contribution is expected to continue, even with a healthy future for natural glycerin.

The second product area which is shared by petrochemicals and oleochemicals is detergent-range (C12-C18) alcohols. These alcohols can be combined with ethylene oxide to form surfactants which display performance advantages in many detergent applications. Technological and marketing efforts over the last 15 years have resulted in dramatic growth of capacity to produce the alcohol portions of these surfactants. Capacity has, for the most part, been based on synthetic chemistry utilizing various types of ethylene growth reactions. In recent years, ca. 85% of such alcohol production has been based on this chemistry in the USA. World production has been ca. 65%, as shown in Figure 11. Alcohols in this range derived from natural sources come principally from coconut and palm kernel oils. These natural feedstocks are expected to remain available for alcohol production and will certainly continue to be used in the future. We believe, however, that competition for coconut and palm kernel oils in world food markets, security of ethylene feedstock supplies and ease of management of olefin coproduct slates will result in continued major dependence on petrochemical supplies of these alcohols during the next decade.

The third product area currently served by the PCI and OCI is that of linear short-chain fatty acids. Production of linear fatty acids by the PCI in the United States is limited to  $C_5$ ,  $C_7$  and  $C_9$  chain lengths. They amounted to ca. 20% of the total US linear acids produced in this range in 1980. Ca. 15% of world production, excluding the Eastern Block, is estimated to be from synthetic sources, as shown in Figure 11. The extent to which demand evolves for the specific properties of narrow cut synthetic acids will determine their future competitive position. Growth of the synthetic lubricant market is believed to be the most important key to overall demand growth for these products. Until such high performance demand materializes, the outlook remains more favorable for the oleochemical industry where these acids can be produced economically in the modest volumes needed and in an acceptable balance with other coproducts.

Closely linked to the fatty acid market are the detergentrange  $(C_{12}-C_{18})$  fatty amines. In 1980 in the USA, ca. 80% of the  $C_{12}$ - $C_{18}$  fatty amines produced came from fatty acids. The remainder were manufactured from petrochemical-based detergent alcohols and  $\alpha$ -olefins. World production is similarly more heavily based on OCI sources as shown in Figure 11. Unless demand for the fatty amines expands faster in the future than anticipated, we believe this ratio of PCI and OCI supply sources will not change significantly. As in the previous cases, products based on petrochemicals are preferred in applications where precise control of hydrophobe chain lengths and purity are critical.

Thus, in those product areas where opportunities exist for significant substitution, factors other than feedstock prices are important. In the areas which have been discussed, it seems unlikely, however, that products from the PCI will capture significantly greater market share than they have today. The petrochemical industry will continue to provide a stabilizing influence in supply-demand balances. In addition, should accelerated demand occur in any of these markets, technology and resources available in the PCI will allow it to meet the demand without coproduct burdens. Thus, end users can depend on the availability of these products on a large scale and therefore plan for the long term.

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## Development of New Crops for Industrial Raw Materials

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#### ABSTRACT

Commercial fats and oils are still used extensively in chemical manufacturing processes, but their fatty acid compositions are limited in variety. An extensive screening program for potential new oilseed crops has led to the discovery of many good sources of new lipid classes and fatty acids. Among them are long-chain acids (Crambe, Limnanthes, Lunaria), medium-chain acids (Cuphea, Umbelliferae, Lauraceae), hydroxy acids (Lesquerella), epoxy acids (Vernonia, Stokesia), acids with special unsaturation (conjugated; acetylenic;  $\Delta 3$ ,  $\Delta 5$ ,  $\Delta 6$ ,  $\Delta 17$  monoenes) and liquid wax esters (Simmondsia). Many of these plant species have received further attention in terms of germplasm collection and evaluation; breeding and agronomic studies; and processing and utilization research on oil and byproduct meal. Some have been developed sufficiently for early commercialization. Recent history has shown this last step to be the most difficult. No satisfactory mechanism has been devised as yet to simplify the process of transferring research information on a developed new crop to reach the ultimate goal of sustained, large-scale commercial production. Close cooperation between governments and private sector institutions, with some financial support, may be required for the first few years to achieve successful commercialization.

#### INTRODUCTION

Earlier reviews on USDA's long-term research program in the search for and development of new industrial oilseed crops have centered around the screening of uncultivated plant species, and plant breeding and agronomic efforts to upgrade wild germplasm to manageable crops (1-4). Other aspects of this program include chemical and engineering research necessary to convert harvested seed crops to highquality commodities, in this case oil and meal; and research to identify prospective users or to adapt new oils or derivatives to existing raw material streams. The latter areas involve research, exploring the feasibility of new bulk products and studies on the often unique chemical and physical properties of unusual lipids that reside in the botanical store house.

Existing processing technology was developed for a select few commercially produced oilseeds, principally: soybean, sunflower, cottonseed, peanut, linseed, rapeseed and palm species. Processing parameters are well established to reduce these crops to high-quality oils and valuable byproducts. All of the commercial oils are made up of the glycerides of a select few fatty acids (Table I); and their stability during processing is sufficiently understood to guard against hydrolysis, oxidation or other detrimental deterioration. For new oilseed crops, existing equipment and processes can be useful, but often proper parameters have to be established to produce acceptable products.

Similarly, new seed oils that can be produced domestically need testing to prove their merit as replacements for