Chapter 4

CATALYST PERFORMANCE TESTING

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4.1 INTRODUCTION

The ultimate objective of a catalyst testing program is the evaluation of the catalyst for performance in a commercial process. Development of the catalyst usually begins with small samples tested in laboratory-scale equipment. It is, of course, desirable that the testing results from such small equipment simulate with considerable accuracy the performance in a large-scale commercial unit. The characterization of a catalyst in terms of its activity is obviously a qualitative measure of the ability of the catalyst to carry out a particular chemical transformation under specified conditions. Speed of reaction and specificity or selectivity are prime considerations. Testing of a catalyst for activity implies a range of experiments varying widely in the degree of sophistication of both the experimental equipment employed and the interpretation of information obtained (Anderson, 1985). It is therefore necessary to distinguish clearly what information is required and to what ultimate use it is to be applied. According to Anderson and Pratt, the most common objectives are:

- Routine quality control tests conducted by the manufacturers or users of a catalyst which may involve a reaction carried out under standardized conditions on individual batches or samples of a particular catalyst type.

- Rapid screening of a large number of catalysts to establish an order of merit for a particular reaction. Such experiments are often carried out in relatively simple apparatus and under mild conditions. Interpretation may be based on the determination of a single reaction parameter.

- More detailed comparison of several catalysts. This may involve testing under conditions covering the likely range of commercial application to identify the optimum performance area of each. Evaluation may be based on a number of criteria, and the resistance to known poisons and the reaction atmosphere determined.

- The determination of the mechanism of a specific reaction, possibly involving the use of labelled molecules and sophisticated analytical equipment. This information may assist in the formulation of a suitable kinetic model or provide valuable clues in the search for improved catalysts.

- The determination of the detailed kinetics of a reaction over a particular catalyst. The kinetics of deactivation or regeneration could also be of interest. This information may be needed to enable the design of a commercial plant or demonstration unit to be performed.

- The continuous long-term operation of the catalyst in such a way as to simulate commercial reaction conditions. It is usually performed in a reactor having a similar configuration to the planned commercial system, and may consist of an individual module (for example, a single full size reactor tube) or of a reduced scale version of the full-size reactor.

It is very important to identify at the beginning of a catalyst study the key catalytic problem in a given process. This will determine the correct method of investigation.

Four factors are usually identified as being the most important:

- *Activity*
- Selectivity
- Life
- Cost

While catalyst activity is often emphasized, other properties, such as selectivity, tendency to carbon formation, catalyst stability, poisoning resistance, or the impact of different feedstock characteristics may be more important.

Laboratory testing of a catalyst will usually concentrate on one or more of the first three of the above listed criteria, one of which will be most important for the particular application. Economic factors, while ultimately determining the potential use of the catalyst, cannot usually be obtained from catalyst testing other than from catalyst life data. Catalytic activity can often be defined as the turnover rate or turnover frequency which describes the number of molecules that react per active site per unit time. The problem with this excellent definition is that it is frequently not possible to obtain an exact estimate of the number of active sites on the surface or in the bulk of the catalyst. Other measures in use are: the reaction per unit mass or volume of catalyst; the reaction rate determined in the presence of concentration or temperature gradients; temperature required to obtain a given conversion or yield; reaction conversion of product yield achieved under a given set of reaction conditions; reactant space velocity required to achieve a given conversion or yield at specified conditions; the rate constant derived from a kinetic study of the system (*Catalytica*, 1987).

To determine selectivity it is important to obtain close to 100% material balances. It is also important to identify the by-products and to follow the change of product distribution with time.

Aging of the catalyst with corresponding decline of conversion and/or selectivity will occur in most catalytic reactions. Rates of aging and potential catalyst regeneration to full activity must be investigated.

No catalyst testing is better than the analytical facilities available for analyzing the major product and by-products. Gas chromatography often coupled with mass spectrometry are the most common means of product analysis today. With increasing emphasis on environmental concerns, the need for greater and greater sensitivity of analytical tests has increased. An example of this need is demonstrated by the fact that the sulfur content of fuels 30 years ago was expressed as fractional percentages, whereas it now often required to be in parts per billion. One may expect this trend to continue.

A major problem in testing catalysts for potential use by evaluating them in bench scale equipment is the likelihood of possible heat and mass transport limitations which can occur in large scale equipment and which do not always show up in bench-scale testing. This will be discussed in a later section.

4.2 CATALYST TYPES

There are three major forms of catalysts used in heterogeneously catalyzed reactions:

- pelleted or extruded catalysts
- fluid bed catalysts
- suspension or slurry catalysts

Catalysts used in commercial operation often cannot be used in the same form and size for catalyst performance testing.

In fixed bed commercial reactors, catalyst particle size will often be determined by pressure drop considerations. A test reactor will have a much smaller diameter and probably cannot accommodate the same particle size. Smaller particles will have higher surface area and be less diffusion limited than large particles. Means have to be found to extrapolate from one particle size to another.

Similarly, it is often difficult if not impossible to simulate fluid bed operation in a small bench-scale reactor. Again, there is a likelihood of differences in particle size but also a major difference in catalyst age. While the performance of a fresh catalyst in both commercial and laboratory sized units may be similar, a commercial fluid bed reactor will have a distribution of catalyst particles of different age. This is due to the continuous recirculation of the catalyst after regeneration and to the addition of a small percentage of fresh catalyst. This is very difficult to simulate in a small reactor.

Slurry or suspension catalysts may be simulated reasonably well as far as activity and selectivity are concerned. There are, however, problems of potential catalyst disintegration after extended periods of time which are not likely to show up in relatively short-term tests.

Occasionally it is helpful to study the activity of a single pellet at high mass velocity. This is usually done in a single pellet Berty-reactor with a thermocouple imbedded in the pellet.

4.3 MECHANICAL AND PHYSICAL TESTS OF CATALYSTS

Proper catalyst specifications for mechanical and physical properties are as important as activity and selectivity (Bertolacini, 1989). Poor resistance to attrition and crushing can cause pressure drops and expensive unit shutdowns in refining and petrochemical operations. Setting reasonable specifications depends on the development of reliable test procedures and well characterized reference materials for method development. Statistical control processes can be used to eliminate test variations to reduce off-specification catalysts.

Catalyst stability (Farrar, 1982), attrition resistance (Farrar, 1983), and crushing strength (Farrar, 1984) are most important. Broken catalyst particles in fixed bed reactors cause increased pressure drop by bridging interstices between catalyst particles which can plug the bed with debris. Fixed bed catalysts are prone to breakage when they are loaded into reactors. High pressure, high temperature, and high space velocity feed throughputs exert strain on catalyst particles requiring that catalysts be prepared in different shapes to resist fracture, spalling, and disintegration. Catalyst strength is crucial in tubular cooled or heated reactors, because catalyst breakage will result in maldistribution of flow and overheating (or overcooling) of tubes.

Important tests to measure potential catalyst breakage during operation are single-pellet and bulk crushing strengths. These tests measure the resistance to a compressing force and are used for quality control by the catalyst producer. Bulk crushing measures the ability of the catalyst to support the weight of the catalyst bed. A test is now under consideration for standardization (Bradley, 1988; Bertolacini, 1989). A mechanically driven piston apparatus giving reproducible crushing results has been described by Bearer (1974) as has been a procedure for measuring catalyst attrition resistance (Dart, 1974). Overall, twenty-five standards have been developed by the American Society for Testing Materials, Committee D-32-Catalysts, which include tests for attrition, crushing strength, particle size distribution, and vibrated apparent packing density (*A.S.T.M. Standards on Catalysts*, 1988).

Catalysts in slurry or ebullating bed reactors are subject to attrition. They must resist high turbulence from high gas velocities as well as erosion by solids in the feedstocks. No standard tests seem to have been developed for this particular application.

Fluid bed catalysts must withstand the effects of several thermal stresses during reaction and regeneration. They must also be resistant to attrition in pneumatic lift operation. Their ability to resist excessive sintering is described in a different chapter.

Characteristics of catalysts such as surface area, pore size distribution, crystallinity, metal dispersion, and surface acidity are important parameters which can distinguish good catalysts from bad ones. Tests for these characteristics are described in other chapters of this report.

In general, mechanical characteristics of catalysts are most important for catalysts ready to go into commercial use. In catalyst research for new or improved catalysts, existing or novel processes, activity, selectivity, and life performance will have to be established before it becomes important to test the catalysts for their mechanical characteristics. However, even the best performing catalyst is no good if it cannot stand up to the climate in the reactor.

4.4 ACTIVITY, SELECTIVITY, AND LIFE TESTS

A first objective of catalyst activity and selectivity testing is usually a preliminary screening of a number of new and existing catalysts to establish a ranking of "performance" for a given reaction (*Catalytica*, 1987). Relatively few candidate catalysts need to be investigated beyond this stage. While the initial tests are usually performed in relatively simple laboratory reactors, and the catalyst ranking is often based on a single easily determined performance parameter, it must be kept in mind that the relationship between performance simulation in a laboratory reactor and performance in a commercial reactor is not always well established and is subject to disguises by heat and mass transfer. Preliminary test screening is usually followed by a cursory screening of parameters that affect the reaction, followed by a more detailed comparative evaluation of catalysts with confirmed potential. Dautzenberg (1989) has presented guidelines for an effective catalyst testing program. He emphasizes the importance to define an objective for the catalyst testing program before starting experimentation. A well designed, appropriate experimental strategy will enhance the effectiveness of the program. Statistically derived experimental strategies and a statistical design of experiments will greatly reduce the number of experiments to be performed while providing the desired information.

The choice of an appropriate test reactor is of the utmost importance. Many reactors and their performance characteristics have been described in the literature and are well summarized in Chapter 11 of Satterfield's book (1980) and Chapter 6 in Anderson's book (1985). Anderson *et al.* (1985) state, "Perhaps the most important physical distinction which may be made amongst laboratory reactors is between batch and continuous systems. Nowadays greater use is made of continuous reactors in catalytic studies. It is now relatively rare that catalytic kinetic studies are made in batch reactors, and these systems are mostly used in preliminary screening tests for reactions where high pressures necessitate the use of autoclaves. In such cases catalysts are usually evaluated simply in terms of measured conversion under fixed reaction conditions and reaction time".

Commercial continuous reactors are generally complicated by the presence of several flow modes and radial and longitudinal gradients of concentration and temperature both within and between catalyst particles (Figure 1). In laboratory reactors, however, strenuous efforts are usually made to eliminate these effects in order that information obtained might be absolutely unambiguous. A classification of laboratory reactors taken from Anderson and Pratt (1985) is presented in Figure 2. Reactor selection depends on both the nature of the reaction system under study and the purpose of the work, subject to the constraints of available time and money. A generalized

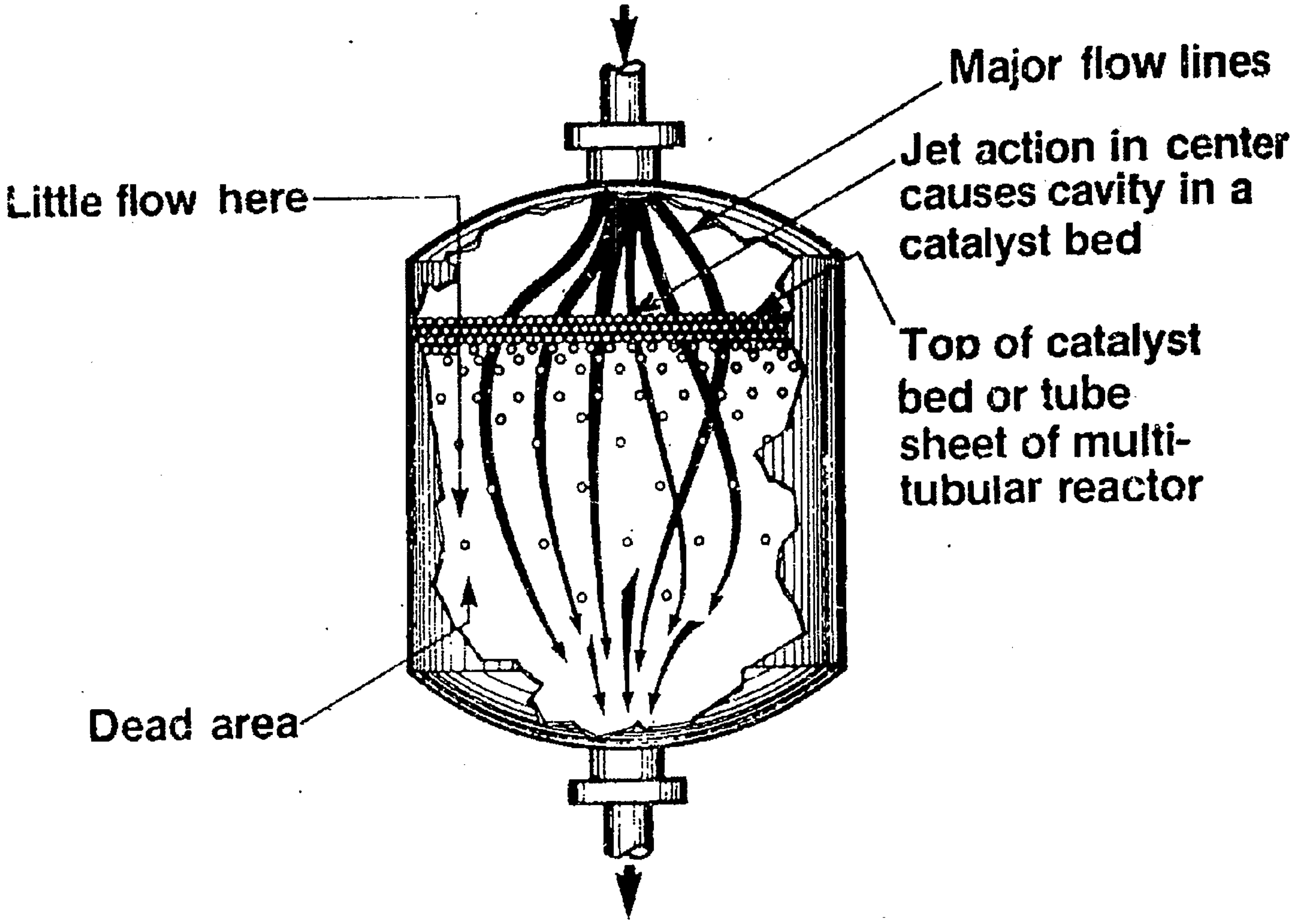

Figure 1. Large Diameter Trickle Reactor with Poor Flow Distribution

(From - F. M. Dautzenberg, 1989

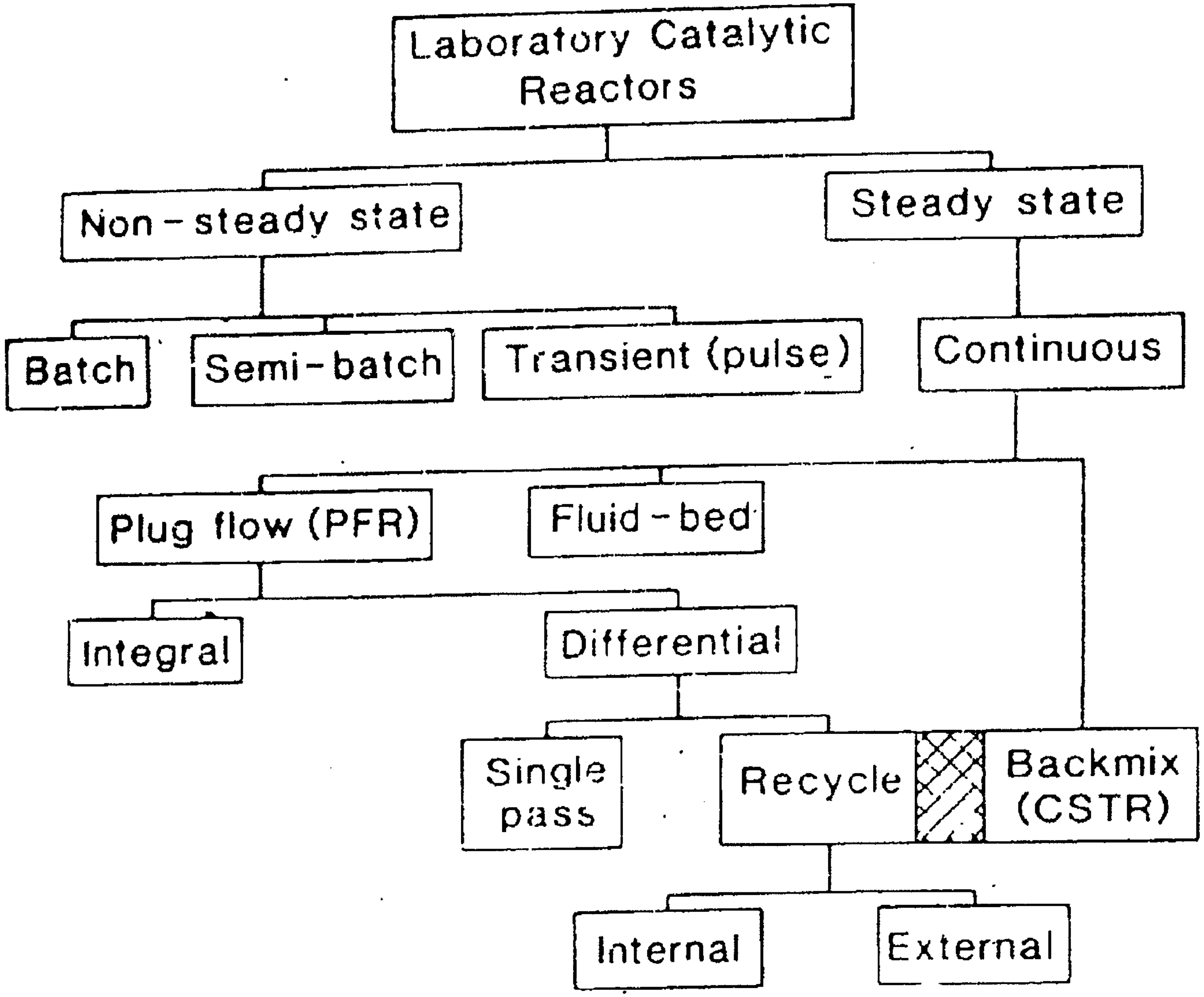

Figure 2. Laboratory Reactors
(From - J. R. Anderson and K. C. Pratt, 1985

preferred reactor selection for different phases of catalyst and substrates is shown in Table 1 (*Catalytica*, 1987). It is always most important to gather the desired information in a reproducible and efficient manner.

It is necessary to have an energy balance, a mass balance for each independent reaction constituent, and a phase balance for each phase of the reaction whether it be gas, liquid, or solid. Isothermal operations simplify the energy balance, and a design is desirable that minimizes pressure drop and is not complicated by the effect of concentration gradients. Continuous rather than batch or semi-batch operation is usually preferred because of the impossibility of uncoupling the main kinetics from deactivation in batch mode and because of the difficulty in defining the actual reaction time in batch operations.

Plug flow reactors and continuous stirred tank reactors are usually preferred over batch or fluidized bed or trickle bed reactors. The complex hydrodynamics in fluidized bed and trickle bed column reactors do not permit an accurate assessment of intrinsic catalyst behavior. However, laboratory trickle bed reactors can be designed to compare catalysts. They are also suitable for life testing of catalyst samples but are generally not good tools for determining reaction kinetics. Methods for evaluating fluid catalytic cracking catalysts have been described in numerous publications, only two of which are referred to here (O'Connor, 1974; Moorehead, 1974). Hydrodynamic properties needed for scale-up of fluidized bed processes can sometimes be obtained from small scale equipment by maintaining strict geometrical similitude and using appropriate dimensional groups for proper scaling (Glicksman, 1984; Fitzgerald, 1984).

The plug flow reactor is particularly efficient for screening solid catalysts in a single fluid phase. The choice of an integral versus a differential plug flow reactor depends on the objectives of the testing. The integral reactor has a number of advantages which make it commonly used. Large conversions reduce analytical problems and lead to more accurate data. Integral reactors are also easy and cheap to build compared to recycle reactors which may be complex. Differential reactors have the advantage that mass and heat transfer influences are usually absent at low conversions and low heat release. Because of the uniform conditions in the bed, most of the parameters of interest can be studied separately. Uniform fluid properties in the bed make true plug flow easier to achieve and in any case, because of the low conversions, the existence of radial velocity profiles does not cause significant departures from the ideals of plug flow. However, because of the small conversions required in a differential reactor, analytical difficulties and therewith the possibility of large errors may arise. While plug flow reactors are preferred for solid-gas and solid-liquid phases, stirred tank reactors are preferable for catalyst screening for solid-gas-liquid phases and for gas-liquid and liquid-liquid phases. A continuous stirred tank reactor is important for evaluation of kinetic parameters and for life tests.

In plug flow reactors gradients in concentration and/or temperature can exist between different locations in the reactor (intra-reactor gradient), between the bulk fluid, and the fluid-catalyst interface (interface gradient), and within the pores of a solid catalyst (intra-particle gradient).

Reactor Selection

	Phases				
Objective	Solid-Gas	Solid-Liquid	Solid-Gas-Liquid	Gas-Liquid	Liquid-Liquid
Catalyst screening	PFR	PFR STR (batch)	STR (semibatch)	STR (semibatch)	STR (batch)
Parameter screening	CSTR	CSTR	STR (semibatch)	STR (semibatch)	STR (batch)
Reaction network characterization	CSTR	CSTR	Trickle bed CSTR	CSTR	CSTR
Kinetic parameters	CSTR	CSTR	Trickle bed CSTR	CSTR	CSTR
Catalyst life tests	CSTR PFR	CSTR PFR	Trickle bed CSTR	CSTR	CSTR
Catalyst optimization	CSTR PFR	CSTR PFR	Trickle bed CSTR	CSTR	CSTR
Scaleup	PFR Fluidized bed	PFR Slurry	Trickle bed Slurry	Bubble column	CSTR
Commercial operation	PFR Fluidized bed	PFR Slurry	Trickle bed Slurry	Bubble column	CSTR
Process improvement	PFR Fluidized bed	PFR Slurry	Trickle bed Slurry	Bubble column	CSTR

PFR	Plug Flow Reactor
STR	Stirred Tank Reactor
CSTR	Continuous Stirred Tank Reactor

Table 1

Assessing the contributions from such gradients requires experimental measurements sometimes supplemented with generalized mathematical criteria. Effective elimination of interferences from the various possible gradients requires appropriate reactor selection, design, and operation. Freedom from transport disguises is an essential criterion for effective catalyst testing in small-scale reactors. Only after the intrinsic catalyst properties are quantified, should the complexities of transfer phenomena be addressed. The ideal reactor is one in which temperature, concentration, and pressure do not vary in space or in time. These conditions are fulfilled completely only in a continuous stirred tank reactor. In a plug flow reactor, isothermal operation is critically important for generating quantitative information about catalyst performance in a laboratory reactor.

Heat transfer coefficients cannot be reproduced in laboratory scale reactors and therefore radial gradients are not observable. It is not enough to study initial rates in gradientless reactors. One must emphasize knowledge of rates at different conversion levels and particularly at close to equilibrium.

Catalyst aging is a phenomenon which can change greatly from catalyst to catalyst. Aging can be caused by different phenomena, such as: accumulation of by-products on the catalyst surface or in catalyst pores (coke); poisons even in very small amounts in the feed; sintering of surfaces at high temperatures; surface rearrangements during reaction; *etc*. Frequently, aging cannot be observed except after fairly long runs. In batch reactors catalyst activity and catalyst decay cannot be independently evaluated. Continuous reactors allow the separation of time scales for reaction and decay. It is also possible to determine changes in catalyst surface and structure by spectrographic techniques. Much work has been done on accelerated aging tests to avoid the necessity of evaluating catalyst performance over long periods of times (days, weeks, or months). One of the best known cases is the steaming of fluid bed cracking catalysts at high temperatures for different periods of time (Satterfield, 1980). However, a great deal of experience is necessary to permit proper correlation between accelerated aging tests and actual aging at normal operating conditions. In reactor tests, aging can usually be observed by changes in conversion and product distribution over a period of time. It is also generally true that most catalysts exhibit different (usually higher) activity when first coming on stream than during a long period of fairly level operation. Of course, this indicates an initial rapid aging probably due to deactivation of specific active sites by poisoning. The most desirable catalytic reactions and catalysts are those that give 100% selectivity to the desired product, thus avoiding interference with a catalyst by by-products formed during the reactions.

In general, it is apparent that catalyst performance testing is a complex, time consuming, and costly effort. It is subject to many pitfalls and must be carried out according to a carefully planned sequence and with careful selection of the right reactor and right operating conditions. In recent years, automation of catalyst testing equipment has enabled workers to test more catalysts on an around-the-clock basis. Combination of computer controlled testing units and computer interacted gas chromatography presents the possibility of obtaining a very large number of data with relatively little manpower requirement. However, it also diminishes direct observation of unexpected phenomena by experienced scientific personnel, and it provides such an abundance of data that it is often difficult to select the important ones and to plot trends.

4.5 MODEL COMPOUNDS

Catalyst characterization can be of considerable assistance in the performance testing of catalysts. The more that is known about the chemical composition and the surface properties of a catalyst, the easier it is to interpret differences in performance between closely related catalysts. This is particularly true for multifunctional catalysts where an understanding of the active sites responsible for specific steps in a reaction sequence will help in interpreting aging and poisoning effects during performance testing. Good understanding will also help in synthesizing new or modifying existing catalysts.

In recent years much emphasis has been put on surface and bulk characterization of catalysts by spectrographic techniques, ranging from infrared spectroscopy, X-ray diffraction, nuclear magnetic resonance, X-ray photoelectron spectroscopy, and many other techniques to quite recent work on scanning tunneling microscopy. This is discussed in a different chapter of this report. However, there are methods of chemical characterization which can throw much light on catalytic mechanisms and therewith on the performance of catalysts. Studies with pure compounds frequently permit identification of specific catalyst sites. This has been demonstrated as early as 1956 for the reforming of petroleum naphthas (Ciapetta, 1958). Dual functionality of platinum-alumina catalysts was first demonstrated using pure organic model compounds to distinguish between acid and metal functions (Mills, 1953). Pines (1960) has published numerous papers characterizing catalysts and their functions by studies of the behavior of model compounds. More recently, the capability of a catalyst has been measured by chemical identification of the bonds which are broken, using a complex organic compound for modeling (Farcasiu, 1991).

While an ideal catalyst will have perfect selectivity, in practice a catalyst produces unwanted products or mixtures of substances. At an early stage in the study of kinetics the existence of parallel and consecutive reaction pathways in chemical reactions can be identified, often by studies with model compounds. The simplest first order rate expressions are then easily integrated to give the variation of product distributions with contact or reaction time. Much more elaborate networks are necessary to describe actual catalytic processes.

Hydrocarbon feeds contain many dozen components, and it is useful to attempt a kinetic analysis in a compromise that acknowledges that different types of organic compounds behave in analogous ways allowing them to be lumped together to give a network similar to that for a pure compound. Development of a network model leans heavily on existing knowledge of catalyst behavior plus experimental work.

The advent of new techniques in surface science has in recent years stimulated much work on an understanding of the structural and chemical properties of surfaces. While the science of catalysis has traditionally advanced as a consequence of new experimental techniques, theory has begun to play an increasingly important role. The availability of powerful computers for extensive calculations has enabled graphical display of results of both experimental surface science and theoretical studies (Salmeron, 1991). This information is becoming helpful in guiding the design of novel catalysts, interpreting experimental measurements, and understanding the way in which catalyst composition and structure affect its activity and selectivity (NRC Report, 1992). *Catalyst by design* is a goal, the attainment of which is gradually becoming more likely. Future catalyst evaluation would be greatly simplified if catalyst performance could be fully predicted from its structural, electronic, geometric, and bond strength characteristics. A major obstacle to this accomplishment will be the difference in temperature and pressure conditions of the surface science measurements and the actual operating conditions during catalytic reactions. It can be assumed that major changes in surface characteristics occur at operating conditions and in the presence of substrates during catalysis.

4.6 ANALYTICAL REQUIREMENTS

As has been discussed earlier in this chapter, almost all catalyst testing for performance in catalytic reactions is being carried out in one of several possible laboratory reactors. The reactions are studied at temperatures and pressures which correspond to those expected to be used in commercial applications and with feed streams which either correspond to those available to industry or simulate components of these feed streams, such as pure organic compounds. Feed streams are metered by volume and weight, as are effluent streams from the reactor. Analysis of feed and effluent streams is usually achieved by gas chromatography, mass spectrometry, and infrared or ultraviolet absorption (Bland, 1967). Fractionation of liquid streams is sometimes required prior to more detailed analysis.

It is essential that excellent mass and weight balances be obtained around the reactor. This may at times require adding an inert internal standard (*e.g.*, a rare gas) to the feed and relating charge components and effluent components to this standard. Since the catalyst may absorb or have deposited on it by-products from the reaction (*e.g.*, coke), it is necessary to have gravimetric analysis of the catalyst before and after reaction as well as identification of the deposits on the catalyst. Only then can a weight balance be complete.

With increasing demand for catalytic processes to control environmentally harmful products and with better knowledge of the effect of very small amounts of poisons on catalysts, it has become necessary to increase the sensitivity of analytical procedures into the parts per billion range. Sulfur analysis, for instance, in petroleum naphtha streams has required continually increasing sensitivity. The analysis of NO_x in combustion exhaust streams prior to and after catalytic reaction also must be in the parts per million range and is usually carried out by chemiluminescence.

New analytical techniques are constantly being developed for greater and greater sensitivity and for components in gas and liquid streams which have not previously been analyzed. New analytical methods will be required in the future as catalytic processes are being developed for environmental control purposes. A particularly difficult consideration is the fact that the concentration of harmful components, which must be chemically reacted with other potentially harmful compounds (*e.g.* NO + ammonia over vanadia-titania catalysts), can be constantly changing and must be monitored continuously to maintain stoichiometry of the reactants.

For conventional catalyst performance testing, particularly of petroleum refining catalysts, units are commercially available which combine reactor testing with gas chromatographic and mass spectrometric analysis of products controlled by integrated computers. Increasing sensitivity requirements make this sort of equipment more complex and consequently much more expensive.

4.7 DISCUSSION

The major part of this chapter is concerned with test procedures of catalysts used in or intended for the petroleum refining, petrochemical, and chemical industries. Existing test procedures which are commonly also suitable for new catalysts involve laboratory tests for the catalyst performance under conditions simulating commercial operations and laboratory tests for the mechanical and physical characteristics of the catalysts. While the performance tests allow selection of superior catalysts for a specific purpose and an evaluation of performance over a range of operating conditions, they are often complex, require expensive testing and analytical equipment, and are time and manpower demanding. Numerous tests are required to optimize the performance of a given catalyst. Since the cost of a catalyst decreases with its increasing life (amount of product formed per unit of catalyst), it is always important to estimate the relative lifetime of competing catalysts. While accelerated aging tests have been developed in many cases, they cannot totally substitute for very long runs in laboratory or pilot plant units. It is easier to extrapolate catalyst life in case of a gradually declining activity than it is in the case of catalyst poisoning, which may lead to feed breakthrough after considerable periods of level onstream production.

A better understanding of the nature of active sites on a catalyst for a particular reaction, of both the number of sites and of site strength, could assist in the development of better performance and life test procedures. A major obstacle to the use of current knowledge in this area is the fact that most observations of surface characteristics are made at conditions which are far removed from those existing during the actual catalytic reaction. In fact, it is likely that the catalyst surface and its active sites at operating conditions and in the presence of substrates differ from those observed at ambient or low temperature and vacuum conditions. There is therefore a major incentive to study catalyst composition, structure, and characteristics at the conditions of the catalytic reaction. Knowledge thus acquired could likely lead to simpler and faster performance tests.

During the last decade or so, there has been a major shift from catalyst research and applications for industrial manufacturing improvements based on profitability alone to consideration of environmental impacts and the use of catalysts in primary prevention of pollution (removal of pollution forming components prior to catalysis) and in secondary prevention (removal of pollutants after catalysis) (Cusamano, 1992). In many cases this trend has required novel sampling and analytical methods. It is expected that, as new processes are developed, new testing and analytical methods will have to follow. It is, of course, impossible to predict the type of tests required unless and until the catalytic process is developed.

Analytical procedures for testing catalyst performance will have to make greater use of more sensitive spectrographic and novel analytical tools. Sensitivity into the parts per billion range will be a requirement in the future; thus, research to develop new instrumentation with this sensitivity will be required.

Modeling of catalyst characteristics and theoretical interpretation of surface and absorbate bonding may eventually lead to a better design of catalysts, and with it to an early understanding of catalyst performance. Research in this direction must be encouraged. As catalysis progresses from an art to a science, prediction of performance should become possible.

4.8 RECOMMENDATIONS

- Research on correlations between laboratory and commercial size reactors to enable faster scaleup time and possibly avoid pilot plant construction.
- Research on accelerated catalyst aging techniques to reduce performance testing time.
- Research on surface properties and diffusional characteristics of catalysts at operating conditions and in the presence of reactants and products to permit deduction to rapid scaleup.
- New analytical techniques will have to be developed to ensure performance testing to meet increasingly severe specifications.

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