Use of Adiabatic Experiments for Kinetic Studies in Fixed Catalyst Beds

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A method is presented for using an adiabatic reactor to study the kinetics of reactions of gases on solid catalysts. The method is based on measurement of the steady state axial profile of temperature or composition in a specially designed adiabatic packed bed reactor. Reaction rates are calculated from these measured profiles by graphical differentiation. The method is applicable for multireaction systems and for any type of kinetic behavior.

The method was demonstrated by an experimental study of cumene cracking on silica-alumina catalyst at 420° to 480°C. The measured reaction rates are in satisfactory agreement with results obtained by other investigators who used isothermal reactors. Areas of application of the adiabatic method are suggested.

The kinetics of heterogeneous reactions are usually measured in isothermal reactors. Frequently however the experimental catalyst bed cannot be kept truly isothermal, especially with systems having large heats of reaction. In such cases significant errors may be introduced if some average temperature is assigned to the isothermal bed, thereby neglecting the effect of temperature variations on the observed conversion. An alternate procedure would be to utilize a method of kinetic study in which an allowance is made for the effects of nonisothermal operation. This may be conveniently accomplished by conducting the experimental study in an adiabatic reactor.

In using adiabatic experiments to study reaction kinetics the basic principle is that the temperature change in an adiabatic reactor may be used to follow the course of a chemical reaction, provided that only one reaction is taking place. This principle is by no means new. It has been used as far back as 1925 to measure the completion time of very fast liquid-phase reactions in a flow system (*7*). However in very few cases have adiabatic methods been used for measurement of the kinetics of chemical reactions. The earliest work is apparently that of La Mer and Read (*10*) who studied neutralization kinetics. Two liquids were rapidly mixed and flowed through a tube equipped with thermocouples to measure the temperature at several axial locations. A maximum adiabatic temperature rise of 0.6°C. was used.

Recently the adiabatic approach was applied to a heterogeneous system by Mars (*12*) who used sliding thermocouples to measure axial temperature profiles in a commercial water-gas shift reactor. Reaction rates were calculated from the slopes of the measured profiles, with axial heat conduction and mass diffusion neglected. The axial temperature profiles differed considerably at different radial positions, so it was necessary to use average values over the reactor cross-section.

Paszthory et al. (*13*) have used another method of studying the rates of heterogeneous reactions, measuring the axial temperature profile in a near adiabatic flow reactor and making an approximate allowance for heat transfer through the reactor wall.

In none of these published studies has an attempt been made to develop the adiabatic method as a tool for laboratory-scale study of the kinetics of heterogeneous reactions. The purpose of the present paper is to describe some experimental and calculative techniques which may be used for adiabatic kinetic studies and to evaluate the relative advantages and limitations of the adiabatic approach. The system considered is a gas mixture flowing through a fixed bed of porous catalyst pellets.

ONE-REACTION SYSTEMS

A one-reaction system is here defined as a system in which only one chemical reaction occurs. This reaction is presumed to have a significant enthalpy change. In such a system the steady state axial temperature profile in an adiabatic reactor is a unique measure of the progress of the reaction. For kinetic studies it is only necessary to measure the axial temperature profile; reaction rates and composition profiles can be calculated from the temperature profile.

Measurement of Reaction Rates

Consider an adiabatic packed bed reactor in which there are no radial variations in fluid velocity, temperature, or composition, that is one-dimensional flow in the axial direction. For a one-reaction system the energy balance for steady state operation is

$$G\,C_P\,A\,\rho_S\frac{dT_G}{dw}-K_e(A\,\rho_S)^2\frac{d^2T_G}{dw^2}+r_k\Delta H_k=0 \quad (1)$$

where the respective terms represent changes in bulk gas temperature, axial heat conduction, and chemical reaction.

If the axial profile of T_G vs. w is measured and plotted as a smooth curve, numerical values of (dT_G/dw) and (d^2T_G/dw^2) can be obtained by graphical differentiation. The value of r_k at any axial position can then be calculated by algebraic solution of Equation (1) with a literature value of K_e. Once the point values of r_k are obtained at known conditions of temperature and composition, they may then be tested for a fit to any postulated kinetic expression.

Adiabatic Reaction Path

For a single chemical reaction taking place in a flow reactor with negligible axial heat conduction or mass diffusion the mole fraction y_k of any reaction participant is related to the gas temperature T_G by

$$y_k = \frac{y_{k_0} + M_0 \left(\frac{C_P}{\Delta H_k}\right)(T_G - T_{G_0})}{1 + \delta_k M_0 \left(\frac{C_P}{\Delta H_k}\right)(T_G - T_{G_0})} \tag{2}$$

The terms ΔH_k and C_P are assumed to be constant.

Equation (2) is valid for any type of reaction kinetics and can be considered as a definition of an adiabatic reaction path. The term δ_k is a stoichiometric factor which accounts for changes in total moles of gas due to chemical reaction. For a reaction having the stoichiometry

$$aA + bB + cC \rightleftharpoons dD + eE + \ldots \tag{3}$$

the parameter δ of a reactant or product would be defined, respectively, as

$$\delta_A = \frac{a + b + c - d - e - \ldots}{a} \tag{4}$$

$$\delta_E = \frac{a + b + c - d - e - \ldots}{-e} \tag{5}$$

Equation (2) is used to calculate the bulk gas composition corresponding to each computed value of r_k.

Use of Equation (2) to calculate y_k's from T_G does not wholly neglect the effects of axial heat conduction or mass diffusion. It assumes that the effect of axial mass diffusion on the y_k vs. w profiles is the same magnitude as the effect of axial heat conduction on the corresponding T_G vs. w profile. This will usually be true, since most of the heat conduction occurs by the same turbulent diffusion mechanism as the axial mass diffusion. If use of Equation (2) is not justified, an iterative procedure can be used (*18*) to calculate the gas composition.

Calculation of Rate Constants

By the foregoing procedure a single experimental temperature profile gives several values of the reaction rate r_k, each at known conditions of T_G and the y_k's. These r_k values may then be tested for a fit to any postulated kinetic expression. For example the kinetic expresesion to be tested might be taken as pseudo m order:

$$r_k = F(P_T y_{kS})^m \exp\left(-\frac{E_{ac}}{RT_S}\right) \tag{6}$$

Since the catalytic reaction occurs on the solid, Equation (6) is properly expressed in terms of conditions at the solid surface (T_S, y_{kS}). These conditions may be computed from the bulk gas properties (T_G, y_k) in the usual manner, with literature values (*2*) of heat and mass transfer coefficients.

Taking the logarithm of Equation (6) one obtains

$$\ln\left[\frac{r_k}{(P_T y_{kS})^m}\right] = -\frac{E_{ac}}{R}\frac{1}{T_S} + \ln F \tag{7}$$

Therefore a plot of numerical values of the left-hand side of Equation (7) vs. $1/T_S$ will be linear if Equation (6) is a valid representation of the rate expression and the correct value of m has been assumed. Different kinetic expressions may be tested in this manner, and the expression which gives the best straight line is chosen as the best representation of the data. The constants E_{ac} and F are then calculated from this line.

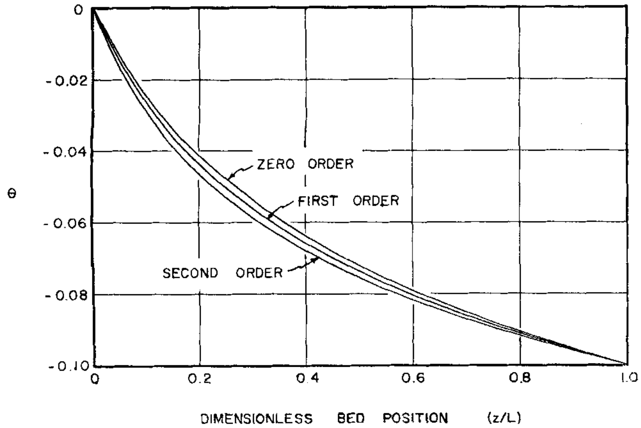

Fig. 1. Effect of reaction order on shape of axial temperature profile.

When the postulated kinetic expression contains more than one temperature dependent parameter, for example the Langmuir-Hinshelwood type of equations, the method for calculating constants is more complicated. One approach is to conduct several experimental runs covering approximately the same temperature range but at different total pressures and compositions, and then to calculate constants by comparing the r_k values at any selected T_S. This presumes that changes in total pressure do not affect the form of the rate expression. This procedure was used in the cumene cracking study [Equation (9)].

As the complexity of the kinetic expression increases, the precision of each calculated constant decreases, so a very complex expression is justified only when the precision of the experimental data is very high. In general the adiabatic method can give sufficiently accurate data so that overall reaction rates can be correlated with an accuracy of ± 10% or better. However the results are not particularly suitable for determining individual parameters in complex kinetic equations, because of insufficient precision of the data and because the coupled temperature-composition relationship makes it impossible to change just one variable at a time in order to measure its separate effect on reaction rate.

Sensitivity of Method to Reaction Order

The effect of reaction order on the shape of the axial adiabatic temperature profile is shown in Figure 1 for a typical endothermic reaction with 20% conversion. These curves were calculated from analytical solutions (*5, 18*) of the adiabatic energy balance for the case of negligible axial heat conduction and $T_G = T_S = T$. The shape of the axial profiles is not very sensitive to reaction order, even for this rather large conversion. For smaller conversions the difference in curvature would be even less.

Because different reaction orders give similarly shaped profiles, a single experimental profile does not give a very accurate measure of the reaction order. This can be shown by considering the first-order profile in Figure 1 as experimental data and by testing these data for a fit to zero-, first-, and second-order kinetics, as shown in Figure 2. The plots in Figure 2 are all closely approximated by straight lines; therefore it is not possible with a single experimental profile to determine the correct reaction order, even to the nearest integral value. Moreover a single profile gives only an approximate value of E_{ac}, since the slopes in Figure 2 depend on the assumed m.

This insensitivity of an axial profile to reaction order is a result of the functional relationships in the system, and not of the method of calculation. The insensitivity in the adiabatic case is quite analogous to the situation in an integral isothermal reactor, when "even complex catalytic systems approximate a pseudo first-order relationship when only space velocity is varied" (*8*). Normalizing the abscissas in Figure 1 is mathematically equivalent to changing the space velocity, and the result is to bring the zero- and second-order curves quite close to the profile for first-order kinetics, that is close to pseudo first-order behavior.

Since at least two experimental adiabatic profiles are needed to provide a good estimate of reaction order and activation energy, it is desirable to obtain two profiles which will give maximum precision for the calculated rate constants. At any given temperature level this is usually best accomplished by varying the total pressure as widely as possible between the two runs. In the analytical solutions for axial temperature profiles (*5, 18*) the effect of total pressure P_T on conversion is very sensitive to reaction order. This procedure assumes that the form of the rate expression does not change with pressure level. An alternative experimental procedure is to use an inert diluent to vary partial pressures at constant P_T; however diluents are generally undesirable because they can cause significant differences in kinetic behavior (*1*).

MULTIREACTION SYSTEMS

In a multireaction system the axial composition profiles are no longer unique functions of the temperature profile and cannot be calculated from temperature measurements alone. For kinetic analysis in a multireaction system it is therefore necessary to measure the axial composition profiles directly, by sampling along the reactor. From these data the local reaction rates may be obtained and tests of postulated kinetic expressions carried out.

DESIGN OF EXPERIMENTAL ADIABATIC REACTORS

In the preceding discussions of the adiabatic method it was assumed that a one-dimensional model could be used for the adiabatic bed, that is that radial variations were negligible in the experimental reactor. In order to meet this requirement while working with a small, laboratory-scale reactor, a special configuration of the catalyst bed was proposed and tested (Figure 3). The catalyst charge was separated into a series of short cylindrical sections, supported on screens, with baffled spaces for gas mixing and temperature measurement or sampling between adjacent sections. This configuration has several advantages which make it useful for both adiabatic and nonadiabatic experiments.

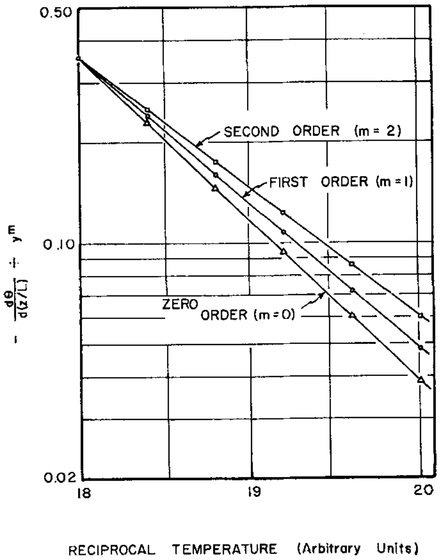

Fig. 2. Test for reaction order.

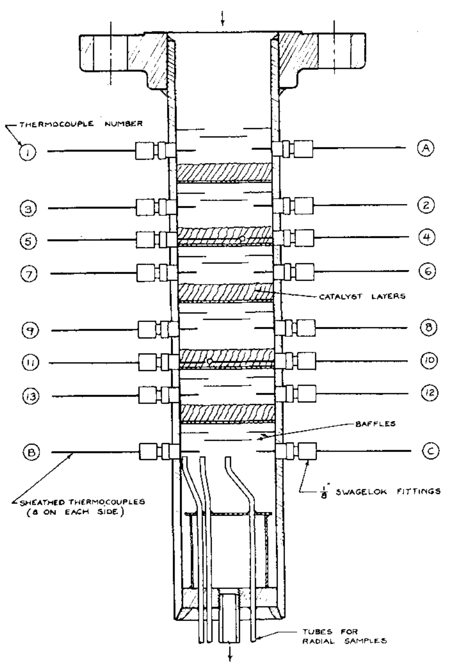

Fig. 3. Experimental reactor.

1. A smaller bed diameter may be used, with attendant lower feed consumption. Even though velocity profiles in each catalyst section are not flat, the baffles prevent cumulative build up of radial temperature and concentration gradients from one section to the next. Therefore the separated bed may be treated mathematically as a one-dimensional system.
2. The separated bed simplifies the problems of obtaining average composition or temperature measurements over the reactor cross section at any chosen axial position.
3. By varying the thickness and spacing of the catalyst sections the designer has considerable flexibility in choice of conversion level and in the location of axial thermocouples or sampling points.

In any one section the radial velocity variations will give rise to a distribution of fluid residence time, but this will generally have a negligible effect on conversion because the conversion per section is small.

The boundary conditions in the separated bed are taken such that a plot of T_G vs. w is a smooth curve. This assumption is valid if there is no significant heat exchange with the reactor wall, if there is no homogeneous chemical reaction and if there is negligible axial heat conduction in the gas spaces.

EXPERIMENTAL STUDY OF CUMENE CRACKING

The adiabatic method was used to study the cracking of cumene to benzene and propylene on porous silica-alumina catalyst spheres at 420° to 480°C. This reaction was chosen to demonstrate the adiabatic procedure because cumene cracking is a simple one-reaction system (*15, 19*), because the catalyst activity is constant and reproducible (*15*), and because the kinetics had been studied extensively by other investigators using isothermal beds (*4, 11, 16, 17*). The enthalpy change due to the cracking of pure cumene at 460°C. is 22,690 lb. centigrade units/lb. mole.

Feed Materials and Catalyst

The cumene feed stock analyzed 98.1% cumene, the balance comprising several different aromatics and naphthenes. The original cumene contained 0.07 wt. % cumene hydroperoxide, a strong inhibitor for cumene cracking (*16, 21*). The hydro-

TABLE 1. CATALYST PROPERTIES

Weight % Al_2O_3	10
Surface area, sq. m./g.	415
Average bead diameter, mm.	3.81
Packed density, g./cc. bed volume	0.71
Particle density, g./cc.	1.18
Real density, g./cc.	2.40
External void fraction	0.40
Void fraction inside beads	0.51
Pore volume, cc./g.	0.432
Average pore radius, Å.	20.8
CAT-A activity index	46

peroxide content was reduced to 0.0009 wt. % by silica gel adsorption treatment (*15*) before the cracking tests.

About 20 wt. % of reagent grade benzene was added to the feed in some of the runs to evaluate the inhibiting effect of benzene on the reaction rate.

All sample analyses were made by gas chromatography except the analysis for cumene hydroperoxide, for which iodometric titration (*20*) was used.

The catalyst was a sample of white bead catalyst purported to be the same as that used in other published studies of cumene cracking (*4, 17*). A —5 to +6 mesh fraction of unbroken spherical beads was used in the experimental runs. Catalyst properties are given in Table 1.

EXPERIMENTAL APPARATUS

The equipment layout is shown in Figure 4. Liquid feed was pumped through an electrically heated vaporizer which provided a superheated feed for the adiabatic reactor. The reactor effluent gas, consisting of benzene, propylene, and unreacted cumene, was condensed and cooled to about 7°C. The liquid condensate, which contained all of the cumene and benzene and essentially all of the propylene, was collected for analysis. Uncondensed gas was vented through a wet test meter. Air could be supplied to the reactor for regenerating the catalyst and nitrogen for purging.

All equipment which came into contact with the hot gas was constructed from stainless steel, principally type 304. Other lines were copper or brass.

The experimental reactor (Figure 3) was a vertical 18-in. long piece of 2½-in. diameter schedule 40 pipe, flanged at the top and sealed at the bottom. The five catalyst sections were each supported on a removable support plate-baffle assembly, shown in Figure 5. The legs of this assembly rested on a screen covering the next lower catalyst section.

Sixteen 0.040-in. O.D. sheathed chromel-alumel thermocouples were inserted into the reactor through fittings in the pipe wall. Twelve were used to measure the axial profile of gas temperature, which was the primary determination of reaction rate, and four were used to find the difference between gas temperature and the temperature inside individual catalyst pellets. This was done by inserting the tip of one thermocouple snugly into a drilled out hole in a catalyst bead and positioning a second thermocouple outside the surface of this same bead. Small corrections were made for heat conduction along the thermocouple sheaths.

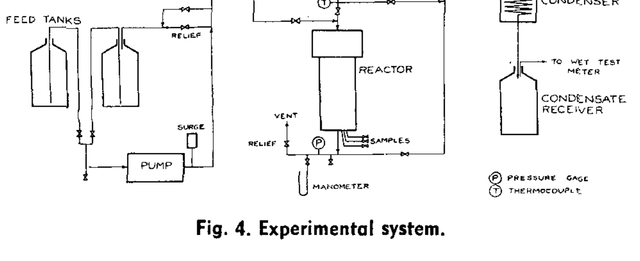

Fig. 4. Experimental system.

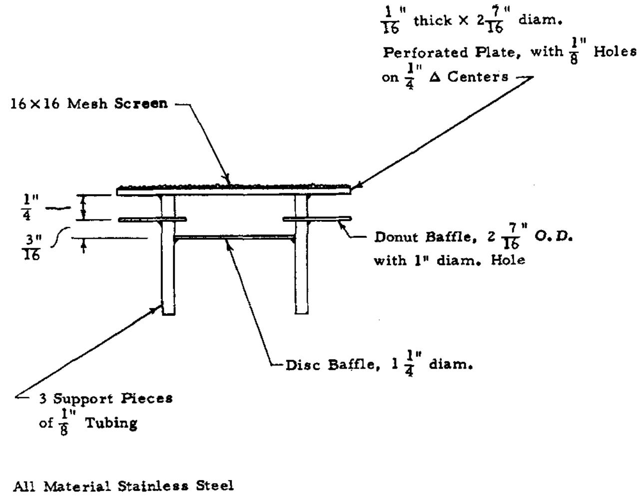

Fig. 5. Support plate and baffle assembly for reactor.

The reactor was covered first by a 1-in. layer of hydrous calcium silicate pipe insulation, over which were wound two concentric coils of heating wire, separated by asbestos tape and covering the central portion of the reactor where the catalyst was located. One of these coils had a constant-pitch winding, the other a pitch which increased with bed length, from top to bottom. The power inputs to these two coils were regulated manually to keep the axial temperature profile in the 1-in. insulation essentially equal to the corresponding axial temperature profile inside the reactor. This procedure eliminated radial heat transfer through the reactor walls, and thereby permitted the catalyst bed itself to operate adiabatically. Additional coils were used to heat the portions of the reactor above and below the catalyst section. All heating coils were covered with an additional 3 in. of insulation.

Thermocouple A (Figure 3) was used as a reference, and its reading was recorded directly. For each of the other fifteen thermocouples inside the reactor the difference between thermocouple temperature and reference temperature was measured, with a precision of about 0.2°C., by bucking the electromotive force values. About 4 min. were required to read and record the fifteen positions, with a hand-balancing potentiometer. To avoid errors from stray currents it was necessary that the hot junction and the sheath be electrically insulated from each other in the reference thermocouple, but not in the other thermocouples.

Tests showed that the disk-and-donut baffles gave sufficient mixing so that the thermocouples located below the baffles would measure essentially the average gas temperature over the reactor cross section.

Operating Procedure

At the start of each run the reactor and vaporizer were purged with nitrogen and heated electrically to the desired temperatures. A spare cumene feed tank was used to bring the vaporizer to steady state at desired flow and temperature, bypassing the reactor to avoid excess coking on the catalyst. Then purified cumene was fed through the vaporizer to the reactor.

The catalyst activity was high at the start of each run (*15, 16*) but levelled off after 40 min. and then remained constant for at least another 100 min., and probably longer. All of the kinetic measurements were made during this period of constant catalyst activity. In each run the feed rate was kept constant, and bed temperature profiles were recorded at several pressures. With each temperature profile a sample of reactor effluent was taken for analysis, to confirm that operation was adiabatic. The feed rate used varied slightly from run to run over the range of 12.56 to 13.07 lb./hr.

After each run the system was purged with nitrogen, and the catalyst bed was regenerated (*16*) with air at 500°C. This procedure gave reproducible catalyst activities from one run to the next.

The cumene cracking rate was measured over the range 420° to 480°C., 1 to 3 atm., and 0 to 0.35 mole fraction benzene. All measurements were made on a single 86.1-g. catalyst charge. In any one run the maximum conversion was 12 mole % of the feed, and the maximum adiabatic temperature drop of the gas was 37°C.

The experimental temperature measurements were sufficiently precise so that smooth axial profiles could easily be drawn through the data points (Figure 6). It was possible to measure the slopes of these profiles with sufficient precision so that the resulting profiles of (dT_G/dw) and (d^2T_G/dw^2) vs. w were all smooth.

The measured axial ΔT_G differed by an average of 8% from the ΔT_G calculated for adiabatic operation from the product analysis. There is evidence that these discrepancies were caused mainly by random analytical errors. It was assumed that reactor operation was sufficiently close to adiabatic conditions to permit calculation of reaction rates from the temperature profiles. This assumption seems justified by the final results, which show no tendency to deviate in proportion to discrepancies in the energy balances.

In catalytic cumene cracking the main products are benzene and propylene. In this work the only significant side reaction was the exothermic, equilibrium-limited formation of diisopropylbenzene isomers. The heat effect of this side reaction was 1 to 7% of that of the main reaction, and a suitable allowance was made in the calculations. The diisopropylbenzene equilibrium becomes much more favorable at lower temperatures, and cumene cracking cannot be considered a one-reaction system at temperatures much below 400°C. Tests showed diisopropylbenzene formation to be nearly 50% of the main reaction at 333°C. Therefore the cumene cracking results of Prater and Lago (*16*) cannot be considered as a true kinetic correlation in the region 300° to 400°C. because the effects of two reactions are in fact superimposed.

EXPERIMENTAL RESULTS

The benzene formation rate was correlated satisfactorily by the kinetic expression

$$\text{Rate} = \frac{k K_C P_C}{1 + K_C P_C + K_B P_B} \qquad (9)$$

where

$$k = (1.08 \times 10^5) \exp\left(-\frac{37{,}000}{R T_S}\right) \qquad (10)$$

$$K_C = (1.0 \times 10^{-14}) \exp\left(\frac{46{,}000}{R T_S}\right) \qquad (11)$$

$$K_B = (1.3 \times 10^{-7}) \exp\left(\frac{22{,}000}{R T_S}\right) \qquad (12)$$

These parameters describe the apparent kinetics observed on a given size catalyst bead exhibiting severe pore diffusion effects, not the true kinetics of the reaction at the catalyst surface. These experiments were carried out to test the ability of the adiabatic technique to provide local rate data. For this purpose correlation in the form of an expression for the apparent kinetics is satisfactory. Studies of the true kinetics can be carried out by the adiabatic bed method. If this is to be done, a range of catalyst sizes should be used, including catalyst particle sizes so small that pore diffusion is not important.

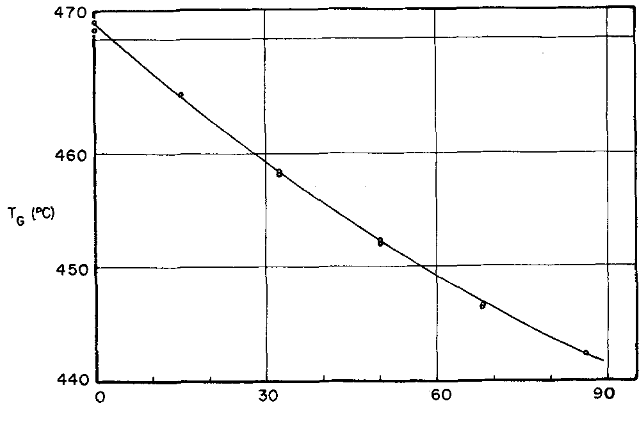

Fig. 6. Typical experimental profile in reactor.

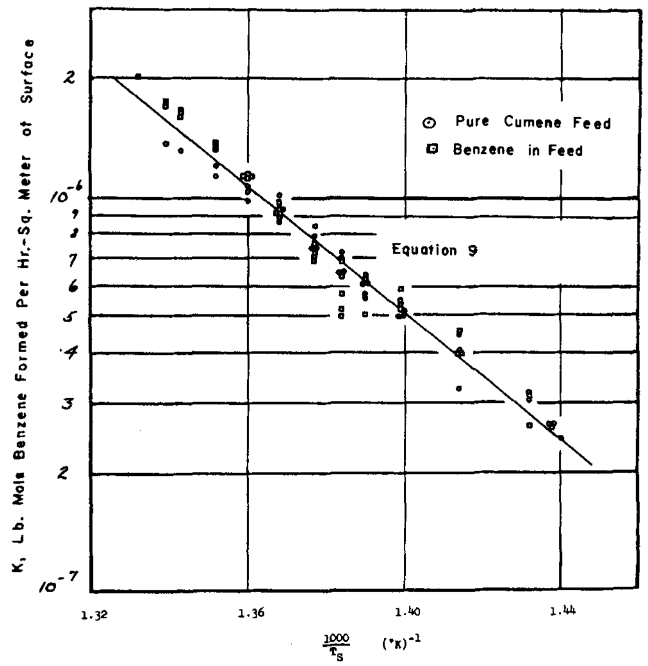

Fig. 7. Correlation of rate constant *k*.

The given values of K_C and K_B are probably not very accurate; the calculation of these constants involves differences between large numbers and is very sensitive to small errors in the rate data. The effect of temperature on K_C is probably too high in Equation (11). The calculated values of k for all experimental runs are shown in Figure 7. Each of these points was calculated from a single measured value of the reaction rate by assuming that K_C and K_B were correctly represented by Equations (11) and (12). The k data exhibit the customary Arrhenius effect of temperature on the rate constant. The fit of the calculated points to a straight line confirms that Equation (9) gives an adequate description of the overall reaction rates, even though the values of the individual parameters may not be very accurate. The 95% confidence limits for the parameters in Equation (9) are

$$k = F \exp\left(-E_{ac}/RT_S\right)$$

where

$$F = (1.08 \pm 1.1) \times 10^5$$

$$E_{ac} = 37{,}000 \pm 1{,}600 \text{ lb. centigrade units/lb. — mole}$$

The fit of Equation (9) to the experimental data should not be taken as confirmation of any type of surface rate mechanism, because the results are complicated by pore diffusion effects (*21*). The effectiveness factor of the catalyst beads used in these experiments was estimated by combining the measured rate data with an analysis of the pore diffusion and surface reaction processes. Values ranging from 0.09 to 0.17 were derived.

The measured cumene cracking rates agree (*18*), within an average variation of about 10%, with rates determined by Rase and Kirk (*17*). These investigators worked with the same type of catalyst and the same bead size, but used an isothermal reactor. This good agreement between isothermal and adiabatic test results confirms the validity of the model and assumptions which were used in the adiabatic method. The cumene cracking results indicate that the proposed adiabatic method of kinetic analysis is feasible on a laboratory scale, and that reaction rates can be measured with an accuracy of ± 10% or better.

APPLICATIONS OF ADIABATIC METHOD

It is desirable to study kinetics in differential or integral isothermal reactors whenever possible, because of their simple construction and greater versatility. When these methods will not give accurate results, for example in cases where heats of reaction or activation energies are large, radial gradients are significant, etc., more complex systems must be considered. Alternatives are:

1. The adiabatic method.
2. A steady state recirculation method (*14*), in which a pump is used to recycle most of the reactor effluent back to the inlet of an isothermal reactor operating with differential conversion per pass. Small amounts of make-up feed are continuously added, and like amounts of reactor effluent are continuously removed.
3. An unsteady state recirculation method (3), in which the time rate of concentration change is measured as a batch of material is continuously recycled through an isothermal bed.
4. A reactor equipped with a piston turbulence generator (*9*), in which high velocities past the catalyst surface are achieved by a piston which pushes gas back and forth through a small isothermal bed, while small amounts of fresh feed are added and product withdrawn.

All four of these methods avoid the problems in temperature control and conversion measurement that arise with the simpler once-through isothermal reactors. A comparison of these four methods shows that the adiabatic approach has the following advantages:

1. Elimination of the need for a pumping device that will operate at system conditions without introducing leakage, adsorption, or catalytic problems.
2. No problems from side reactions caused by recycle of products.
3. Ease of measuring reaction rate of pure feed, unmixed with recycled products.
4. Reduction in the number of chemical analyses, since temperature measurements are used to follow the course of the reaction (one-reaction system).
5. More information obtained per run, since a single run gives some estimate of activation energy.

The principal limitations of the adiabatic method are that the reactor configuration is somewhat complex, and that catalyst activity must remain constant until steady state adiabatic operation is achieved. In addition it is not possible to change one variable at a time to study its separate effect of reaction rate because of the coupled relationship between temperature and composition.

NOTATION

A = total reactor cross section, sq. ft.

C_P = heat capacity of gas mixture, lb. centigrade units/lb.-°C.

E_{ac} = activation energy for rate constant, lb. centigrade units/lb.-mole

E_z = axial mass diffusion coefficient based on total bed cross section sq. ft./hr.

F = frequency factor for the reaction rate constant

G = mass velocity based on cross-sectional area of empty reactor, lb./hr.-sq. ft.

ΔH_k = heat of reaction due to disapperance of 1 mole of component k, lb. centigrade units/lb.-mole

k = apparent reaction rate constant, lb.-moles/hrs.-sq. m. catalyst surface

K_e = axial thermal conductivity of bed based on total bed cross section, lb. centigrade units/hr.-ft.-°C.

K_B, K_C = adsorption coefficients of benzene and cumene in apparent kinetic equation, atm.$^{-1}$

L = axial length of bed

m = order of reaction

M = average molecular weight of gas mixture

P_B, P_C = partial pressures of benzene and cumene, atm.

P_T = total pressure, atm.

r_k = molal rate of disappearance of component k due to chemical reaction, lb.-moles/hr.-cu. ft. bed vol.

R = gas constant, 1.987

T = combined temperature of gas and solid, °K.

T_G = temperature of gas, °K.

T_S = temperature of solid, °K.

w = weight of catalyst, measured from reactor inlet, g.

y_k = mole fraction of component k in bulk gas

y_{kS} = mole fraction of component k in the gas at the catalyst surface

z = reactor length in the axial direction

δ_k = defined by Equations (4) and (5)

θ = $T - T_o/T_o$

ρ_S = weight of catalyst per unit bed volume, g./cu. ft.

ρ = molal gas density, lb.-mole/cu. ft.

Subscripts

j, k = values referred to components j and k

o = value measured at reactor inlet

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