Kinetics of Propane Pyrolysis

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A kinetic model based on the most important free radical reaction steps has been developed for propane pyrolysis. The kinetic and product distribution data were obtained over a wide range of conversions at temperatures from 700 to 850°C. and with various amounts of steam or other diluents. The results of the investigation clarify the important reaction steps and the effect of the critical operating variables.

Although the pyrolysis of propane is used for large-scale production of ethylene and propylene, the kinetics and mechanism for the reaction are not yet completely understood. The rate of propane pyrolysis has frequently been reported to be first order relative to propane concentrations, especially at lower conversions of 40% or less (*4, 11*). Both Crynes and Albright (*3*) and Buekens and Froment (*1*) have recently shown however that the overall rate is not well described by either first-order or other simple-order equations.

Pyrolysis reactions of propane and other light hydrocarbons always involve a complicated series of consecutive and simultaneous free radical steps (*7* to *9, 13, 14, 19*). At low conversions, approximately equal moles of ethylene, propylene, methane, and hydrogen are produced when propane is pyrolyzed (*3, 5, 10*). Several of the primary products and especially propylene are relatively unstable. As propane conversions increase, yields of ethylene and methane increase relative to those of propylene and hydrogen (*1, 3*). Ethane, butenes, butadiene, aromatics, heavier components, and acetylene are always produced to at least a small extent. The surface of the reactor is also known to effect the pyrolysis reactions to at least some degree (*3, 12, 18*).

Because of the complexity of the reaction mechanism, it is not surprising that simple order kinetic equations are not applicable. Considerable questions still exist though as to just which free radical steps are important in the overall processes for the various light paraffins.

Many previous pyrolysis investigations have been at operating conditions quite different than those used commercially. Temperatures and pressures employed have often been relatively low, and the rates of pyrolysis were then much less than those in commercial units. Although steam is apparently employed exclusively as a diluent commercially, it has been employed only to a very limited extent in kinetic investigations reported to date.

Snow et al. (*15, 16*) have recently developed a mechanistic kinetic model for representing quite satisfactorily the data for ethane pyrolysis. This model is based on what are likely the most important free radical steps. Rate constants for each reaction step were expressed as a function of temperature by the Arrhenius equation. The pre-exponential terms and the energies of activation used are in the range reported in the literature. This specific kinetic model must be considered rather preliminary in nature, however, since the kinetic data available for ethane pyrolysis do not appear to be completely consistent. Furthermore, the model does not contain terms for some less important reaction steps. Current literature does not contain adequate kinetic data for propane pyrolysis in order to develop a similar mechanistic approach. Such data have now been obtained in the present investigation. A mechanistic model that represents the kinetics of the reaction and predicts product composition has also been developed.

EXPERIMENTAL DETAILS

The equipment used in this investigation was the same as that used by Crynes and Albright (*2, 3*) except for the following features:

1. Tubular flow reactors were constructed from ¼-in. O.D. 20 gauge 304 stainless steel tubing. Reactors used were either about 40- or 175-in. long.

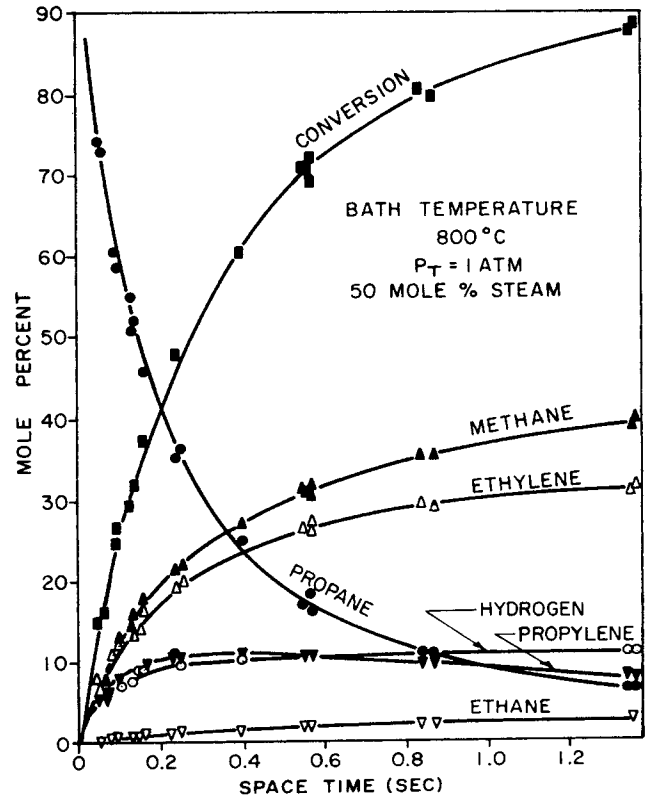

Fig. 1. Product distribution versus space time at 800°C. and with 50% steam.

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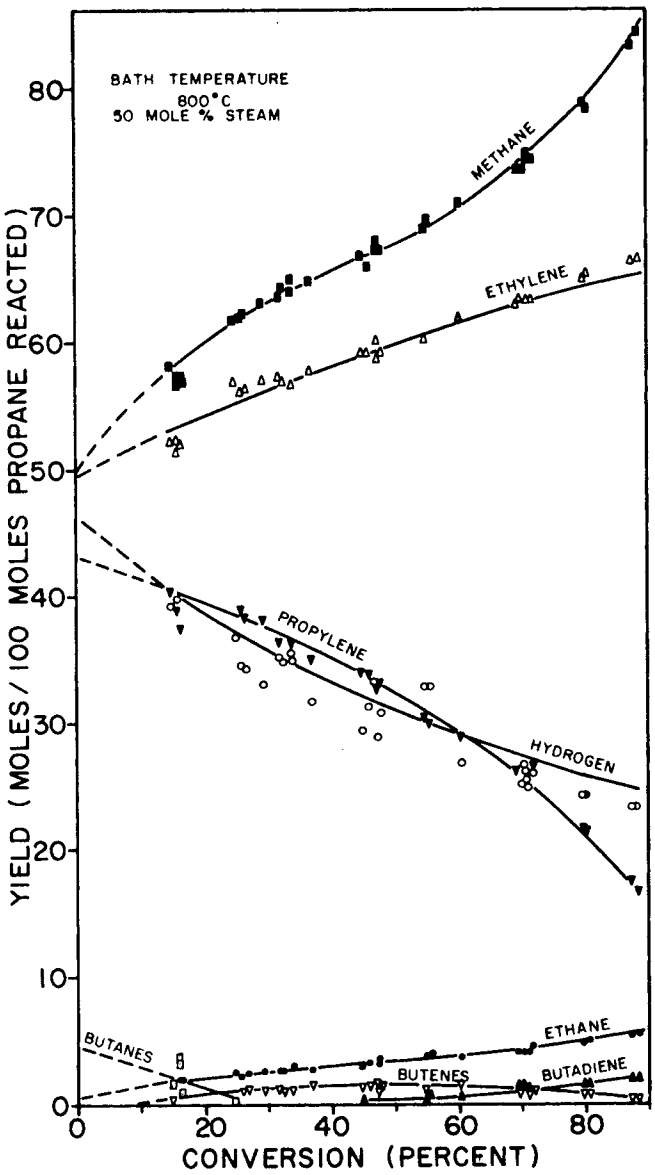

Fig. 2. Product yields versus conversion at 800°C. and with 50% steam.

2. The reactors were immersed in a fluidized sand bath rather than in a molten lead bath. The four chromel-alumel thermocouples placed at different points in the sand bath usually read within 5°C. of each other.

3. The propane feed gas was saturated in some runs with steam by bubbling the propane through hot water. The amount of steam in the entering gas mixture was adjusted to either 25 or 50 mole %.

4. The effluent gas stream from the reactor was dried by passing it first through a 0°C. trap and then through granular calcium sulfate. The dried product was analyzed with the gas chromatograph used by Crynes (2) for hydrogen and hydrocarbons through C_4's. Several samples were analyzed on another gas chromatograph for C_4 through C_6 hydrocarbons. These latter analyses were made primarily for products obtained at higher conversions.

Table 1 summarizes the bath temperatures, steam concentrations, and propane conversion levels investigated. Bath temperatures of essentially 700, 750, 800, and 850°C. were employed and the total pressure in the reactor was always approximately 1 atm. Spaces times from 0.04 to 6 sec. were obtained in this investigation by varying the reactor length and/or flow rate. The space time was calculated by dividing the reactor volume by the total volumetric flow rate of the feed mixture at the reactor inlet pressure and at bath temperature. Thermocouple measurements of the gas stream in both the entrance and exit sections of the reactor were made. The effective reactor volume was assumed to be that portion of the tube at essentially the bath temperature. Readings in the gas stream throughout the reactor indicated larger temperature differences between the bath and the gas stream as the rate of endothermic pyrolysis reactions increased. Although the thermocouples were subject to some conduction and radiation errors, the approximate level of these errors can be estimated by comparing the readings made during pyrolysis with those made when inert gases such as nitrogen or helium were passed through the reactor. Temperature differences between the bath and the gas were probably 15°C. or even higher in many cases for pyrolysis runs at 850°C. but were considerably less, 5°C. or less, at 750°C.

Conversions of propane and yields (moles of product formed per 100 mole of propane reacted) were calculated in the same manner used by Crynes (2). In general, the carbon, hydrogen, and overall material balances around the reactor agreed within 1 to 2%, except for runs in which considerable heavy ends or carbon were formed. Analyses from duplicate runs were used to calculate the reproducibility of the experimental data. The standard deviations for single ethylene and propylene yields are 0.8 and 1.1% respectively on an absolute basis. Similar

TABLE 1. OPERATING CONDITIONS AND PROPANE CONVERSION LEVELS INVESTIGATED

Steam concentrations, mole %	Bath temperature, °C. 700	750	800	850
0 (untreated reactor)	7-34%	18-65%	23-85%	30-96%
0 (H_2S treated reactor)	7-65	22-38	25-66	—
25	—	10-84	15-93	27-66
50	8-17	12-81	15-88	23-78

TABLE 2. REGRESSION EQUATIONS FOR THE YIELDS OF THE VARIOUS PRODUCTS

$$Y = b_0 + b_1X_1 + b_2X_2 + b_3X_3 + b_4X_4 + b_{11}X_1^2 + b_{22}X_2^2 + b_{12}X_1X_2 + b_{33}X_3^2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{14}X_1X_4 + b_{111}X_1^3 + b_{112}X_1^2X_2 + b_{113}X_1^2X_3$$

where

Y = yield (moles of particular product/mole propane reacted)
X_1 = fractional conversion of propane
X_2 = (temperature °C. − 800)/50
X_3 = mole fraction steam in feed
X_4 = { 0 untreated reactor; +1 hydrogen sulfide treated reactor }

	Ethylene Reg. coeff.	Propylene Reg. coeff.	Ethane Reg. coeff.	Methane Reg. coeff.	Hydrogen Reg. coeff.
b_0	0.52146	0.43309	0.00015	0.54282	0.41557
b_1	0.08705	−0.15776	0.14866	0.52073	−0.29211
b_2	0.00217	−0.01890	0.00530	−0.00338	0.03438
b_3	−0.04752	0.03387	0.02051	−0.09005	0.08980
b_4	—	—	−0.00127	−0.01075	0.01394
b_{11}	0.01780	0.03667	−0.16103	−0.93027	0.13171
b_{22}	−0.00585	−0.00353	0.00378	−0.00242	0.01664
b_{12}	0.03097	0.01774	−0.03025	−0.01149	—
b_{33}	—	−0.05429	−0.01458	—	—
b_{13}	0.31175	−0.13400	−0.10980	0.34203	−0.09863
b_{23}	−0.00982	—	0.00805	−0.00867	—
b_{14}	0.02896	—	—	0.04178	−0.09162
b_{111}	—	−0.23693	0.10260	0.87522	—
b_{112}	—	—	—	—	—
b_{113}	−0.20794	0.16946	0.06908	−0.34737	—

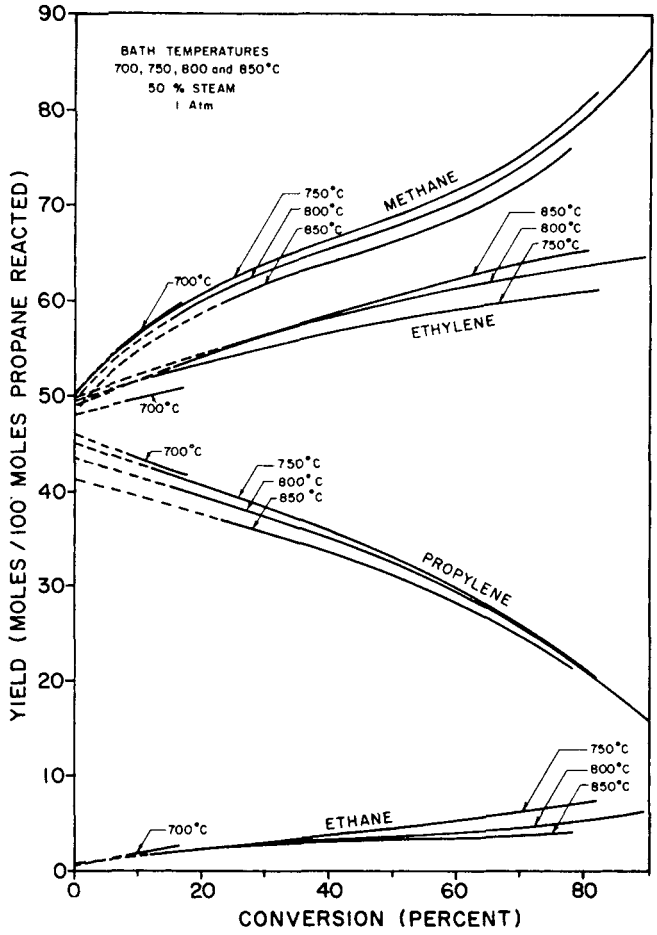

Fig. 3. Product yields versus conversion for various temperatures using 50% steam.

values were obtained for other products, except for hydrogen that had a standard deviation of 3.1%.

KINETIC AND PRODUCTION DISTRIBUTION RESULTS

At each of the four temperature levels (see Table 1), three levels of steam were investigated over a range of space times. Figure 1 shows the conversion and distribution of the major products as a function of space time for several duplicate runs made at 800°C. and using 50 mole % steam in the feed stream. Methane and ethylene yields were significantly greater than those of hydrogen and propylene especially at higher space times (and also higher conversions). The results of Figure 1 were used to calculate the yields of the various products as shown in Figure 2. The yields of all main products and also the minor ones (ethane, butane, butenes, and butadiene) varied significantly with the propane conversion. Yields of aromatics (not shown on Figure 2) increased from about 0.04 to 0.6% as the conversions increased from 65 to 94%.

Yields of the major products were found to vary significantly with temperature, amount of steam in the feed mixture, propane conversion, and the pretreatment of the inside walls of the reactor. The yield of each of the major products is expressed as a function of these four independent variables by empirical equations summarized in Table 2. The general form of these equations is given, and under each product the coefficients of the significant terms are listed. Statistical analyses of the regression equations indicate that the lack of fit of the equations are similar in value to the experimental errors caused by repeated experiments, and it can be concluded that the equations are good descriptions of the experimental results. The solid lines shown in Figure 2 and all following figures are the predicted yields obtained for these equations. Figure 2 is an example of the comparison of the data and the predicted yields. Experimental data are not plotted on the subsequent figures in order to maintain clarity.

Figure 3 illustrates the effect of temperature on product yields over the range of conversion investigated when the feed stream is 50 mole % steam and 50 mole % propane. The yield of ethylene increases with higher temperature, especially at high conversions. Propylene yield decreases with increasing temperature, and this effect is greatest at low conversions where propylene yields are the highest, about 40%. Methane yields climb from near 50% at low conversion to above 80% at high conversion, and the effect of increasing temperature is rather uniformly to decrease the yield. The low ethane yield increases with conversion but decreases with temperature. Temperature trends similar to those shown in Figure 3 were noted when less steam was used in the feed stream.

Figure 4 illustrates the effect of the amount of steam on the yields of the various products when operating at 800°C. Greater amounts of steam increase the ethylene yield, especially at high conversions. Propylene yield is decreased only by about 1% by adding 50% steam. Methane and ethane yields are likewise decreased by about 1% at the higher conversions. Since hydrogen yield lines intersect those for propylene yields, in order to maintain clarity they are not shown in Figure 3 and 4. On a weight basis, the hydrogen yields are low. The 95% confidence limits of the predicted ethylene yields are indicated at several points on Figure 4, and are of the magnitude of

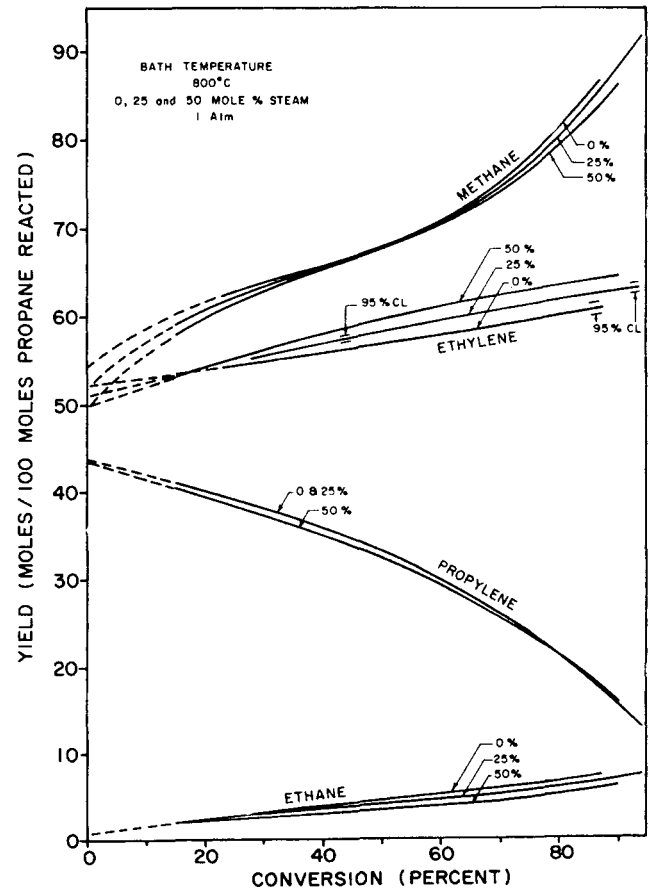

Fig. 4. Product yields versus conversion for various steam concentrations at 800°C.

± 0.5 to ± 0.7% depending upon the reaction conditions.

When no steam was used as a diluent, the reactor tended to plug rather quickly, often in a matter of minutes at higher temperatures, 800°C. and especially 850°C. Increased levels of steam dilution minimized plugging; when 50% dilution of propane was used at 850°C., the reactor was operated for periods of several hours without any noticeable plugging problems.

When the reactor was treated with hydrogen sulfide, such treatment caused a small increase in the ethylene yield for runs in which no steam was added as a diluent. No significant changes in ethylene yields were noted for runs made using steam nor in propylene yields for runs made with or without steam.

Although conversion was treated as a pseudoindependent variable in the above presentation of the results, in reality it is a dependent variable. Figure 5 shows how the conversion varies with space time, temperature, and steam. High conversions are of course reached much more rapidly at high temperatures. At a given temperature and space time the conversion depends upon the amount of steam with the propane feed. Increasing the steam concentration always raises the conversion and the higher the temperature the greater is this effect. At 800°C. an increase of about 8% conversion is caused by addition of steam to the extent of 50%.

Several factors probably cause this steam concentration dependency:

1. Space time is greater than the actual residence time of the gases in the reactor since the actual moles of gases increase with conversion. The residence time is relatively more nearly equal to the space time as the fraction of steam in the feed increases.

2. Since pyrolysis is highly endothermic, the steam acts as a heat sink so the actual temperature of the reacting gases is higher and is relatively more nearly equal to the bath temperature.

3. As will be discussed later, the initiation reaction which is reversible is important in determining the overall rate of the reaction. This reaction is first order in the forward step and second order in the reverse step, and the overall rate of initiation is increased as the partial pressure of propane is decreased or as the steam concentration is increased for a constant total pressure.

Several runs were made using helium or nitrogen as the diluent instead of steam. Helium results were essentially identical with those using steam. Therefore steam apparently does not act as a third body or interact chemically with the reactant gas. Steam does however reduce the partial pressure of the propane which, for example, as shown earlier, enhances the ethylene yield. It also removes coke deposits from the walls of the reactor. Decreased rates of coke deposition were observed whenever steam was being added, and carbon oxides were noted in the effluent stream. The carbon oxides were obviously formed by water gas reactions.

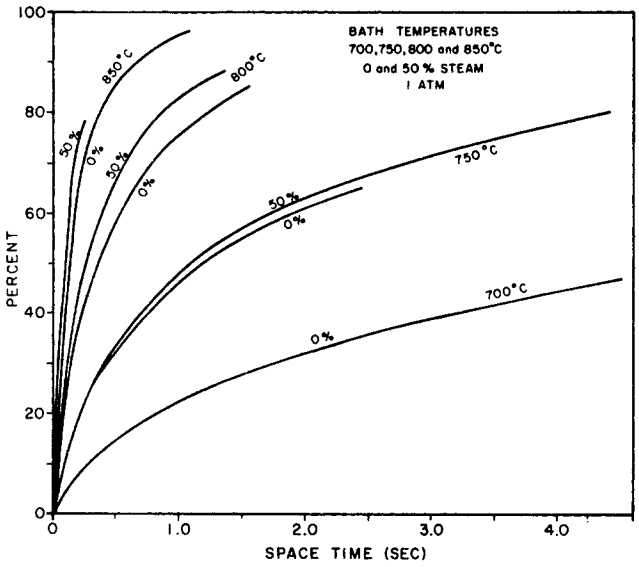

Fig. 5. Conversion versus space time for various bath temperatures and steam concentrations.

Pyrolysis runs using nitrogen as the diluent must be considered preliminary in nature since the reactor rapidly plugged with carbon. The limited results using 50% nitrogen in the feed indicated that ethylene and propylene yields were 3 to 8% lower but methane and hydrogen yields were higher at 55% propane conversions as compared to the results for steam runs. The lower yields of olefins probably resulted because of the increased importance of secondary reactions which produced coke.

Effect of Surface Treatments

Additional information was obtained concerning the effects of treating the inside walls of a reactor with hydrogen sulfide and other gases. Crynes and Albright (*2, 3*) had earlier reported results indicating the importance of such treatments in affecting the course of pyrolysis. Contacting hydrogen sulfide with the reactor for several minutes at temperatures from at least as low as 100° to 800°C. resulted in metal sulfide films on the reactor walls.

The sulfide surface is relatively effective in preventing the formation of metal oxide surfaces when oxygen or steam is contacted with the reactors. Steam when contacted for periods of 6 to 24 hr. with reactors that had been treated with hydrogen sulfide slowly converted some of the metal sulfides to metal oxides. These metal oxides promote coking reactions and the formation of larger amounts of hydrogen. In general, the length of time to convert sulfide surfaces to oxide surfaces was longer for reactors that had been used for an appreciable period of time as compared to relatively new reactors.

This investigation confirmed qualitatively that reactor history is a fairly important factor in the overall pyrolysis process since it affects the types of heterogeneous wall reactions which are especially important relative to coke (or carbon) and hydrogen formation. Although the exact roles of the surface are not known, the inside surfaces of the reactor were roughened considerably and the reactors became embrittled as the reactor was used. Such changes were undoubtedly caused by a combination of oxidation steps, carburization, etc. which resulted in chemical changes of the surface.

Kinetic Modeling

The experimental results of this investigation for propane pyrolysis are considered to be much more complete and accurate than any previously reported. The results furthermore cover the entire temperature range of commercial importance, and they should be most useful for developing a mechanistic kinetic model such as developed by Snow et al. (*15, 16*) for ethane.

Some but not all of the key free radical steps for ethane pyrolysis are important for propane pyrolysis. As a result, portions of the model used by Snow et al. can be used in the one for propane pyrolysis. The main initiation step for ethane pyrolysis is the following

$$CH_3CH_3 \rightleftarrows 2CH_3\cdot \qquad (1)$$

In propane pyrolysis, the above reaction is certainly of considerable lesser importance because the concentration of ethane present is always relatively small and especially

because the C—C bond in ethane is much stronger than those in propane (*17*). The key initiation step for propane pyrolysis must certainly be as follows:

$$CH_3CH_2CH_3 \rightleftarrows CH_3CH_2\cdot + CH_3\cdot \qquad (2)$$

Breaking of a C—H bond in propane is of limited importance as an initiation step because the C—H bond is stronger than a C—C bond in the propane.

Snow et al. (*16*) used a trial-and-error procedure in devising a kinetic model for ethane pyrolysis. They tested their model using various combinations of free radical reactions since there is no general agreement as to the most important reaction steps. They also tested various values of A and E to be used in the Arrhenius equation ($k = A\,e^{E/RT}$) for expressing the k values for each reaction step as a function of temperature. A similar trial-and-error procedure was adapted in the present investigation.

For a tubular plug flow reactor at constant total pressure in which essentially two moles of products are formed for each mole reacted (as was experimentally noted in the present investigation), differential equations of the following type describe the system

$$\frac{dC_i}{d\tau} = \frac{C_r}{C_{r0}(1+X)} \sum_{j=1}^{m} a_{ij} r_j - C_i \frac{dX}{d\tau}$$

$$i = 1, 2, 3 \ldots . n$$

where

$$r_j = k_j \prod_{\substack{i=1 \\ a_{ij}<0}}^{n} C_i^{-a_{ij}} - k'_j \prod_{\substack{i=1 \\ a_{ij}>0}}^{n} C_i^{a_{ij}}$$

It was initially assumed in making the calculations that the reaction was at isothermal and isobaric conditions. After a rather detailed trial-and-error procedure, the model shown in Table 3 was solved using a CDC 6500 digital computer and was found to describe the pyrolysis results of propane for temperatures from 700 to 850°C., for partial pressures of propane from 0.5 to 1.0 atm., and for propane conversions up to 70%. Briefly the program used to solve the model as described by Snow (*15, 16*) is divided into two periods. During the induction period which lasts only a few milliseconds for propane pyrolysis, all the differential equations are directly integrated. After the induction period, the steady state assumption is applicable, and it was used throughout the rest of the integration.

Table 3. Propane Pyrolysis Rate Constants as Functions of Temperature, $k = Ae^{E/RT}$

Reaction	A	E
I. $C_3H_8 \rightleftarrows CH_3\cdot + C_2H_5\cdot$	6×10^{14}	75
	4.2×10^{13}	0
II. $C_2H_5\cdot \rightleftarrows C_2H_4 + H$	3×10^{11}	35
	7.5×10^{11}	5.4
III. $C_2H_5\cdot + C_3H_8 \rightleftarrows C_2H_6 + C_3H_7\cdot$	4×10^{10}	5
	1×10^{11}	4
IV. $CH_3\cdot + C_3H_8 \rightleftarrows CH_4 + C_3H_7\cdot$	1.5×10^{12}	4.9
	1.1×10^{10}	5
V. $C_3H_7\cdot \rightleftarrows C_2H_4 + CH_3\cdot$	4×10^{10}	32
	3.6×10^{11}	2
VI. $C_3H_7\cdot \rightleftarrows C_3H_6 + H\cdot$	3.6×10^{10}	30
	1.8×10^{12}	1
VII. $H\cdot + C_3H_8 \rightleftarrows H_2 + C_3H_7\cdot$	1.8×10^{11}	4.6
	5.6×10^{9}	8
VIII. $C_3H_7\cdot + CH_3\cdot \rightarrow C_3H_6 + CH_4$	1×10^{14}	0

The consumption of materials for the formation of free radicals is assumed to be negligible compared with that for the formation of molecular products. Thus the $dC_i/d\tau$ are essentially equal to zero in equations for which the C_i is the radical concentration. These equations then become implicit algebraic equations which are solved for the free radical concentrations at each integration step by a general Newton iteration procedure. The differential equations are numerically integrated using the Milne four-point predictor-corrector method.

The values of the frequency factors (A's) and activation energies (E's) which were found to best describe the pyrolysis of propane over the entire range of temperatures are given in Table 3. The calculated results were not very sensitive to several of the rate constants, particularly the reverse rate constants for reactions 3, 4, and 7. Thus the values given for these constants probably are subject to the most doubt.

The activation energies (E values) reported in Table 3 tended to be in the lower portion or somewhat below the range of values reported in the literature for the individual reaction steps. Most literature values were determined based on experimental results obtained at less than 200°C., and it is quite possible that activation energies change somewhat with temperature. Frequency factor values (A

Table 4. Comparison of Experimental Results and Values Calculated from the Kinetic Model

	Experimental	Calculated		Experimental	Calculated	
Temperature, °C.	800	790	800	800	790	800
Space time, sec.	0.05	0.05	0.05	0.55	0.55	0.55
Conversion, %	15	16	19	70	65	71
Mole, %						
Hydrogen	5.0	5.5	6.0	11.0	9.5	9.5
Methane	7.5	8.0	9.5	31.0	29.0	31.2
Ethane	0.3	0.6	0.9	1.7	1.0	1.7
Ethylene	6.5	7.0	8.5	26.5	28.0	28.7
Propane	75	73	67	18	21.0	17
Propylene	5.0	6.0	7.0	10.5	10.7	11.0
Temperature, °C.	850	835	850	850	835	850
Space time, sec.	0.04	0.04	0.04	0.18	0.18	0.18
Conversion, %	27	30	38	68	67	76
Mole, %						
Hydrogen	9.0	7.5	8.1	13.7	9.5	9.6
Methane	13.0	15.0	18.5	29.5	30.0	32.8
Ethane	0.5	1.0	1.2	1.5	1.3	1.2
Ethylene	11.7	13.8	17.4	26.2	28.5	31.6
Propane	58	54	45	18	18	14
Propylene	8.0	8.5	9.3	10.5	11.0	10.8

values) reported in Table 3 are in poorer agreement with literature values. However, it is doubtful that A and E values are truly constant over the entire range of 200 to 850°C. In fact, some modified Arrhenius equations indicated that A values are temperature dependent.

Product distributions calculated with this kinetic model are in best agreement with experimental values at lower reaction temperatures, particularly at 700°C. Since deviations from isothermal reaction conditions were greatest at high temperature, additional compositions and conversions were calculated for temperatures somewhat below that of the sand bath. Table 4 shows experimental and calculated values for 800° and 850°C. for short and long space times. Conversions and product distributions predicted by the model agree better with the data if the gas temperatures are assumed to be 745°, 790°, and 835°C. in the initial stages of the reaction for bath temperatures of 750°, 800°, and 850°C., respectively. However, for higher conversion levels (near 70%, the upper limit of this model) this temperature trend was not established. In general, the calculated and experimental results agree within the accuracy of the isothermal temperature assumption and the restrictions placed on the reaction products by the stoichiometry of the equations in the model.

Kinetic models in which the temperature varied as a function of tube length would of course be more meaningful in representing the experimental data of this investigation. With such models, it would undoubtedly be possible to choose better A and E values, to choose more effectively the most important free radical steps for the model, and to extend the model to higher propane conversions. Unfortunately sufficiently reliable data for calculating the heat transfer from the reaction wall to the gas stream do not appear to be available. This heat transfer certainly involves both convection and radiation steps. No attempt was hence made in the present investigation to devise a nonisothermal kinetic model.

Several reaction steps which are undoubtedly occurring to some extent during propane pyrolysis include the following

$$C_3H_6 + CH_3\cdot \rightleftarrows C_4H_9\cdot \quad (3)$$

$$C_4H_9\cdot \rightleftarrows C_4H_8 + H\cdot \quad (4)$$

$$C_4H_9\cdot + H_2 \rightleftarrows C_4H_{10} + H\cdot \quad (5)$$

$$C_4H_8 + C_3H_7\cdot \rightleftarrows C_4H_7\cdot + C_3H_8 \quad (6)$$

$$C_4H_7\cdot \rightleftarrows C_4H_6 + H\cdot \quad (7)$$

$$C_2H_4 \rightarrow 2C + 2H_2 \quad (8)$$

The later coking reaction may involve acetylene as an intermediate. Acetylene may also react to form benzene and other aromatics. Ethylene and especially propylene are pyrolyzed to some extent at the temperatures used in this investigation. Recently Kunugi et al. (6) presented a long list of reaction steps that occur during propylene pyrolysis. If additional reaction steps were added to the model shown in Table 3, both the accuracy and the range of the model would presumably be improved.

CONCLUSIONS

A theoretical kinetic model was developed that effectively represents propane conversions up to about 70%. Such a model can undoubtedly be expanded in the future to represent the pyrolysis data for any feed mixture of light hydrocarbons. In order to develop such a model, it will be necessary to obtain reliable pyrolysis data for the specific hydrocarbons to be included in the mixture. Even higher speed computers than are currently available likely will be required for solving such a complex model.

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NOTATION

- A = frequency factor in the Arrhenius expression, sec.$^{-1}$ or cc./(g.-mole)(sec.)
- a_{ij} = stoichiometric coefficient of the i^{th} component in the j^{th} reaction; $a_{ij} < 0$ is a reactant; $a_{ij} > 0$ is a product
- C = concentration, g.-moles/cc.
- C_T = total reactant gas concentration excluding diluent, g.-moles/cc.
- E = activation energy, kcal./g.-mole
- k = forward rate constant, sec.$^{-1}$ or cc./(g.-mole)(sec.)
- k' = reverse rate constant, sec.$^{-1}$ or cc./(g.-mole)(sec.)
- r_j = rate of j^{th} reaction, g.-moles/(cc.)(sec.)
- X = fractional conversion of propane
- τ = space time, sec.
- i = refers to the component, molecular or free radical
- j = refers to the reaction
- m = total number of reactions
- n = total number of components
- o = refers to reactor inlet conditions (including diluent)

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