ABSTRACT

Title of Thesis: Vapor Pressures of Some Coal Oil Fractions

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Thesis Directed by: Dr. D. Zudkevitch, Adjunct Professor of Chemical Engineering

New data on coal tar oils and data from the literature on pure compounds and oils derived from coal were used for testing the predictions by the correlation of Maxwell-Bonnell. Based on the observation that the discrepancies between the predicted values and the data are systematic, recommendations were deduced on needed modifications to the correlation. A proposal for modification to the Maxwell and Bonnell correlation to improve prediction of vapor pressures of highly aromatic fuel fractions with characterization factors of 8 UOPK 10.5 was made.

Experimental data were taken on vapor pressures of fractions of coke oven coal tar oils and of a sample of oil derived from coal liquefaction by the SRC-II process.

Several coal derived oils were separated into fractions in batch distillations. The fractions were characterized and analyzed, and their vapor pressures within the range of 2 to 800 torrs were measured.

A proposed modification for the Maxwell-Bonnell correlation was part of this study.

VAPOR PRESSURES
OF
SOME COAL OIL FRACTIONS

BY

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FOREWORD

The research which has been performed and reported in this thesis deals with studies in Vapor Liquid Equilibrium in Chemical Engineering. A reliable correlation is needed so that process information can be calculated with minimum information input.

Since vapor and liquid equilibrium equipment is scarce at New Jersey Institute of Technology, the equipment and the study was conducted off-site and materials and services were obtained from other sources.

My deepest appreciation is expressed to Dr. D. Zudkevitch for all his help, guidance and support in this endeavor and completion of this thesis. Dr. Zudkevitch not only supplied his expertise in this field but also a large supply of the equipment and samples.

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INTRODUCTION

Processing of chemical and fuel feed stocks from coal derived oils, such as coke oven tars and/or coal liquefaction products, e.g. SRC-II, involve distillation and stripping, absorption and adsorption. Design of these and other processing steps require reliable correlations of data on vapor pressure and other properties of the fractions.

Development of a vapor pressure correlation is an essential part of the preparation of process design data. It has been recognized that use of correlations based upon data on petroleum fractions can introduce large errors when applied to coal derived oil fractions. This can be due to two reasons: one, originally correlated data on petroleum fractions often did not extend to high enough temperatures; and two, coal oil derivatives are more aromatic than conventional petroleum fractions. Because of this, many correlations that have been developed for petroleum process calculations are not directly applicable to designing processing of coal-derived oils and must be modified.

Coal tar oils boil over a wide range of temperatures and contain many chemical compounds. The conventional way to characterize such complex mixtures to develop process design data, is to fractionate the coal tar oil into narrow boiling cuts which can be further analyzed and studied.

Although many reliable procedures exist for correlating the variations of vapor pressure of pure compounds as functions of temperatures, not many are available for predicting these functions from only single known points. Predicting the vapor pressures of mixtures from single, measured or estimated, temperature/pressure points is more difficult and less promising to yield reliable values. Nevertheless, the petroleum industry has been doing just that.

Petroleum crudes and their fractions, natural gasolines and liquids derived from coal are mixtures very crudely defined by their distillation and gravity curves. Other inspections, such as viscosity measurements and concentrations of oxygen, sulfur and nitrogen are also recorded in the assays and are useful in predicting some properties. Still, the variation with temperature of the vapor pressure of a liquid fuel fraction is calculated from only a signle known, or assumed, pressure/temperature point. More specifically, the average temperature for a specific cut of the TBP or ASTM distillation and the overhead pressure of the laboratory distillation column are used together with the cut's gravity for establishing the normal boiling point and other vapor pressure values, as needed, via a generalized correlation such as that of Maxwell and Bonnell.(17)

The Maxwell method which since 1932 has been found very useful and reliable for quite a variety of design computations in petroleum engineering is a Cox-type correlation, where the independent variable is 1/T°R and the dependent variable is the inverse of the absolute temperature (in °R) at which normal hexane has the same vapor pressure as the fraction in question. This correlation in its original form, without corrections, was found reliable for predicting the behavior of paraffinic compounds and petroleum stocks. However, in attempting to predict vapor pressure of aromatic compounds and fuels by Maxwell's method, the need to correct for nonparaffinic-nature was discovered. This led to the later (1955) development of the modified version, by Maxwell and Bonnell (18,19).

The Maxwell-Bonnell Correlation (M-B) includes a correction for deviation from the behavior expected from paraffinic compounds and stocks which have a Watson characterization factor, K, also called UOPK, around 12. The correction, as shown in Figure 6 is applied to the normal boiling point and is emperical. The variables are the known vapor pressure and Watson's K (UOPK).

The instantaneous vapor pressure of a liquid (or solid) fuel sample is that assumed to prevail in a small equilibrium cell, such as the pot or a tray of an Oldershaw or a Sarnia True-Boiling Point (TBP) column. At any time that pressure is:

$$P_F^{\circ}=\sum P_i^{\circ}\ x_i\ \gamma_i \qquad \text{EQ. (1)}$$

where x_i is the mole fraction of component i, P_i° is its vapor pressure and γ_i is its activity coefficient in the liquid phase. P_F° is the vapor pressure of the fuel fraction.

In most cases, fractions of the same stock may be considered to be ideally mixed. Hence, in absence of alternatives, the assumption is made that for all compounds $\gamma = 1$. An example of a case where this assumption was proven valid is given in Figure 1 (30) vapor pressure points of the SRC-II oil of Figure 3 are shown as triangles. The solid curve represents the integral at each temperature of measured pressures of the fractions. Examples of similar computations and conclusions have been published before (8).

Analysis of coal oil fractions (10, 11, 27, 28, 30) have clearly revealed the presence of hetero compounds that definitely do not mix ideally with the predominant hydrocarbons of the liquid fuel. Nevertheless, prediction of the vapor pressures, P_i°, of any individual fraction, even if it is assumed to be a hydrocarbon, is not yet done easily.

Difficulties stem from the type of data, summarized in the "Petroleum Inspection," which are provided to the designer. In essence, the petroleum engineer has only "one point" data to rely on, which is a combination of:

(1) t_i, which is the average boiling point of fraction i collected as overhead at pressure i

(2) ρ_i average density (API gravity) of fraction i if possible at 60°F = 15.5°C or at a given temperature around t_m, the melting point of the cut.

The problem becomes more complicated when data from different experiments, done by different procedures, are to be used to prepare a correlation, or a design.

A. Distillation Data as Source of Single Vapor Pressure Point

Crudes and fractions are usually defined by the curves for distillation and density (or °API gravity), and the viscosities at one or more temperatures. Two types of batch distillations are used in developing the data.

(a) ASTM Distillation - no reflux or packing

- D-86 Atmospheric distillation of gasolines and light ends
- D-158 for gasolines through light gas oils
- D-216 Atmospheric distillation of natural gasolines
- D-285 Crude petroleum
- D-1160 Atmospheric distillation of middle distillates
- D-1160 at 10 mm Hg for heavy oils

(b) True Boiling Point (TBP) Distillation carried out with 15 to 100 trays or equivalent packing and at different Reflux ratios in any of the

- tray types such as the Oldershaw, columns
- Spinning band columns
- Packed columns such as the Sarnia type

The ASTM distillations are simple and standardized. However, interpretations of the data for VLE and other computations is complex. The results from either an ASTM or a TBP distillation are given in the form of Tables and Curves relating distillation temperatures versus % volume off, see upper curve of Figure 2. The ASTM data must be converted to EFV (Equilibrium Flash Vaporization) equivalents before usage for vapor pressure and VLE computations, while the TBP data could be used directly via any "integral" technique (11). In addition, samples are taken at intervals so that their gravities can also be plotted versus % volume off.

More expensive, but necessary for new developments, are the additional tests on carbon/hydrogen ratio and characterization of % paraffins, napthenes, monoaromatics, etc., in each fraction. Sulfur, nitrogen and other hetero-compounds are also quantified.

Each of the samples collected, e.g. 0 -3% off, or 10 to 20% off, can be distilled again to provide another distillation curve. For narrow cuts of naphtha or other mixtures that contain only few constituents, such as the carbolic oil residue, a TBP distillation can include plateaus in the temperture curve, as shown in Figure 4, enabling identification of individual compounds, or azeotropic mixtures, by their boiling points. In all other cases, the number of compounds is so large that tedious procedures would be necessary for separating fractions to individual constituents.

In distillation of either crudes or heavy fractions and residues, it is impossible to continue the atmospheric ASTM or TBP distillation beyond 650°F, lest cracking occurs. Consequently, the distillation is continued in a shorter column under vacuum. Whenever the temperature of 600°F (315°C) which is considered low for cracking, is reached, the overhead pressure is reduced to another level. Thus, a distillation, as shown in Figure 2, is carried out under atmospheric pressure, followed by reduction to say 5 trays and distillation at 50 Torr, which may be followed by distillation without trays and at much lower pressures.

As shown schematically in Figure 2, data from the "short column" vacuum distillation are usually converted via vapor pressure correlations to atmospheric tempertures and plotted as continuation of the atmospheric distillation curve. The conversions are illustrated by the arrows in Figure 2.

For example, and in no relation to Figure 2, a sample taken at 490°F and 10 micron of Hg is recorded as an atmospheric point of 1080°F. This is misleading, since the latter information is derived not measured. Worse, however, is the fact that even at very low pressures, the residues do not boil and the distillation curves terminate after only a certain percentage, e.g. 40% of the original charge has been distilled. The rest is the experimenter's or designer's guess. Recent development on the nature of continuous mixtures may provide for better guesses in the future.

For application of Equation 1 in the manner illustrated in Figure 1, assumption must be made that after conversion from volume fraction to mole fraction, using density-molecular weight correlations, each step represents the concentration, in mole fraction, and the boiling point of either a real or a pseudo compound.

Correlations for petroleum fractions are usuable only for narrow cuts. Therefore, though quite inconvenient, wide cuts, e.g. 200°F wide, are subdivided again into narrow cuts. This is done either in the laboratory or by a computer program that relies on certain assumptions.

The successful application of the method depends on the reliability of the conversion of the TBP curve to a set of pseudo compounds whose VLE K ratios can represent the total behavior. The method of Maxwell and Bonnell (18,19) has been used in the petroleum industry for this purpose.

B. Watson Characterization Factor

Watson and Nelson (28) introduced characterization factor as an index of the chemical character of pure hydrocarbons and petroleum fractions. The charaterization factor of a hydrocarbon is defined as the cube root of its absolute boiling point in °R divided by its specific gravity (60°F/60°F), or

$$\text{K-Characterization Factor} = \sqrt[3]{T_B/\text{Sp. Gr.}} \qquad \text{Eq. (2)}$$

The K value above, also called Watson's K or UOPK, should not be confused with the VLE ration K=y/x. The characterization factor is only an approximate index of the chemical nature of hydorcarbons. However, it has considerable value in that it can be applied to the entire boiling range of a crude and it has been generally accepted by the petroleum industry.

For approximate use when there are insufficient data, several correlations have been developed for typical crude fractions grouped according to characterization factor and viscosity index. These groups are numbered in order of decreasing paraffinicity and each may be considered representative of the crude fractions within its characterization factor or viscosity index range. The five original groups and the additional two groups for aromatic systems were arbitrarily selected as follows:

	Group	Characterization Factor	Viscosity Index of Lube Fractions
Paraffinic	I	12.1	80 - 100
	II	11.9 - 12.2	60 - 80
	III	11.7 - 12.0	40 - 60
Naphthenic	IV	11.5 - 11.8	20 - 40
	V	11.3 - 11.6	0 - 20
Branched Aromatic	VI	10.5 - 11.3	
Highly Aromatic	VII	< 10.5	

II. THE MAXWELL-BONNELL CORRELATION FOR VAPOR PRESSURE

The Maxwell-Bonnell method is applied in the calculation of vapor pressures for pure hydrocarbons and petroleum fractions. Its theoretical base is similar to that of the Cox Chart and utilizes the comparison of the chemical structure, or mixture, to those on n-hexane. Calculations achieve that through the use of the compound's Watson K and the normal boiling point (NBP).

The natural limitations are that this method is only an approximation, and accuracies on compounds other than long-chain or basic hydrocarbons are possibly questionable. Its great advantage stems from that minimum data are needed to perform calculations.

The general Maxwell-Bonnell equation form is:

$$\frac{1}{T_n} = \frac{A_n}{T_6} + B_n \text{ (where } P_n = P_6\text{)} \qquad \text{(Eq. 3)}$$

(Maxwell-Bonnell Equation)

T_n = absolute boiling point of any hydrocarbon above propane.

T_6 = absolute boiling point of n-hexane or
$P_n = P_6$ = vapor pressure corresponding to T_n and T_6
A_n and B_n = constants of the equation.

Calculation of the vapor pressure requires a trial and error approach. This is normally done by a computer. Input to the program is the temperature at which a vapor pressure is desired, the Watson K, and the normal boiling point. An initial pressure is then assumed.

A check is made to insure that the Watson K is between 7.5 and 15.5. If not, or if none has been submitted, a value based upon the component's density at 60°F and its normal boiling point is calculated with Equation 2.

In the program used in this study, calculations abort when all insufficient data options are found non usable.

The dependent variable of Equation 3, $1/T_n$, is a function of the boiling point of a paraffin, i.e. a compound whose Watson K is 12. However, if for the compound's, or the fraction's, K = 12, then an equivalent boiling point of a pseudoparaffin with the same vapor pressure must be used in establishing the A of Equation 3.

In applying the generalized vapor pressure correlation to high speed computers, it is desirable to be able to present it in equation form. The complete equation for the generalized vapor pressure correlation range covered by the charts is:

$$T_B = \frac{748.1A}{\frac{1}{T_p} - .0002867 + 0.2145\ A} \quad (\text{when } P_n = P_6) \qquad \text{EQ. (4)}$$

T_B = normal boiling point of the hydrocarbon, °R (1 atm)

T_p = observed boiling point of the hydrocarbon, °R

A = a function of pressure as defined below:

Pressure level	A Equals	
< 2mm	$A = \frac{4.741 - \log P}{2876.663 - 43 \log P} - 0.0002867$	EQ. (5)
2 - 760mm	$A = \frac{3.877 - \log P}{2387.262 - 95.76 \log P} - 0.0002867$	EQ. (6)
>1.0 atm (760mm)	$A = \frac{4.326 - \log P}{2666.376 - 36.0 \log P} - 0.0002867$	EQ. (7)

P = atmospheres = $P_n = P_6$

The K correction (without the "F" factor) can be represented by the equation:

$$\Delta t = -2.5\ (K-12.0)\ \log\left(\frac{P_2}{P_1}\right) F \qquad \text{(EQ. 8)}$$

Δt = Correction in °F

K = Characterization factor of the hydrocarbon in question

P_2 = Atmospheric pressure

P_1 = Pressure in question in consistent units with P_2

Equation 8 was derived by Maxwell and Bonnell (18, 19) as an empirical correlation of corrections that had been calculated back from data of API RP-42 (2). The grid described by Equation 8 is shown in Figure 6.

For compounds with normal boiling points below 400°F the correction, F, is applicable only to compounds with normal boiling points between 200 and 400°F.

$\text{TBP} < 200°\text{F} \quad F = 0$

$\text{TBP} > 400°\text{F} \quad F = 1$

$$400°\text{F} > \text{TBP} > 200°\text{F} \quad F = \frac{\text{TBP}\ (°\text{R}) - 659.7}{200.} \qquad \text{Eq. (9)}$$

The next stage is a direct reference to the vapor pressure equations of n-hexane. Back-calculating from the initially assumed pressure, a pressure of n-hexane is calculated. Comparison of the newly calculated pressure with the $P_{assumed}$, previously calculated, sets the base for the assumption of a new P. The process continues until internal limits of convergence are met.

Although the Maxwell-Bonnell correlation is extensively used, its users must bear in mind that:

- o The method assumes that the cut is narrow; there are less than 50°F from Initial to End boiling points.
- o The data used for developing the correlation were for paraffinic and

naphthenic compounds, and the correlations for K effects are only first approximations.

- The vapor pressure of a cut is greatly influenced by its front end. In both ASTM-D-86 and TBP inspections, the front end is usually lost and the initial part of the curve, though cherished by the designers, reflects the artistic hand of the laboratory experimenter more than the true nature of the fraction.
- The vapor pressure curve for a mixture is the variation of the latter's bubble point pressure integral as a function of temperature. In contrast with what has been suggested in many publications, most bubble point curves resemble S shape curves rather than straight lines when plotted against 1/T. Therefore, even a narrow cut cannot be expected to follow Maxwell-Bonnell correlation to its critical point. Also, when cuts are mixed, there is so much

overlap that the actual VLE behavior is somewhat different from the predicted integral.

As shown in Figure 5, the correlation for characterization is empirical, and depending on the temperature/pressure of the measured data, the boiling point of the fuel fraction is changed (corrected). It has been questioned (30) whether the two parameters (TBP AND °API) correlation will be sufficient for coal liquids characterization. The problem has many facets; the liquids are rich with polynuclear aromatics, and oxygenated and other heterocyclic compounds, all known to be different in nature from the stocks that were used by Watson, Fenske, Edmister and Maxwell, in developing the correlations.

Preliminary conclusions of an earlier study at Pennsylvania State University (15) suggest the following:

a. Very few data are available, even on the low molecular weight polynuclear and methyl substituted polynuclear aromatics.

b. The little data that are available on aromatics with more than one ring are mostly below 5 Torr.

c. Most compounds are solid through most of the experimental temperature range of most laboratories' apparati. Sometimes extrapolations cannot be accurately made because of sublimation effects.

d. Since for many a compound, neither the boiling point nor the critical properties could be measured, the application of the same correlations yielded differences depending on the reference points used.

e. Predictions of vapor pressures with the Maxwell-Bonnell correlation, as with other correlations, yielded relatively poor results as measured in maximum percent deviation. This, however, could be due to poor quality of data.

In the first phase of this study, vapor pressure data of pure polynuclear aromatics (i.e. vapor pressure curves for phenanthrene, anthracene and carbazole) indicated quite a wide variety of results which could not be acceptable.

Since these results were of such a low reliability, it was felt that experimental data be gathered within the range of interest and then compared to predicted vapor pressures.

III. EXPERIMENTAL WORK

A. Materials

Carbolic Oil Residue - The sample came from Allied Chemical's Detroit Tar plant on July 23, 1980. Light Creosote Oil - The sample came from Allied Chemical's Detroit Tar plant on March 18, 1980.

B. Equipment

1. Vapor Pressure Measurements

a. Vapor Pressure Glass Still

A vapor pressure still jacketed with a hot oil bath was designed, as shown in Figure 26, built and used in all the vapor pressure measurements. It contained a magnetic stirrer, thermowell and a condenser.

2. The Heating System

Two constant temperature baths with internal pumping mechanisms (VWR Haake N3B) within the range of 45°C to 300°C were used for the vapor pressure measurements and the tempered media condenser. In addition to this, for generating more heat, two 17" 1000 Watt

Vycom Corning 16790 immersable heaters were used. Different heating media were used at different temperature ranges of experimentation. Ethylene glycol was used at lower ranges up to 150°C; Dowtherm A was used for intermediate ranges, 150°C - 250°C, and silicon oil was used for high ranges 250°C and above.

3. Pressure, Temperature and Weight Measurements

The barometer that was used was the mercury - Prince Nova fortin-type, scale was 508 mm Hg to 790 mm Hg. Scale readability to ±0.1 mm. A cathetometer was used to read the barometer and differences on the manometer and a McLeod gauge. The latter was accurate to ±0.1 mm Hg.

A Mettler scale beam-balance Model H315 with a built-in weight system was used to weigh each cut. Its accuracy was stated as ±0.1mg. Several thermometers were used in the distillation runs. They were 3" immersion ASTM type with ranges anywhere from -10°C to 360°C with an accuracy of ±.1°C. A Whal digital thermometer Model 1370C with accuracy of ± .2°C and a range from -100°C to 1382°C was immersed in the reboiler. Two Whal digital theremoters were used in measuring the temperature in the vapor pressure measurements.

4. Batch Distillation and Preparation of Samples

The distillation was done with a 20 plate 1" Oldshaw column with a liquid splitter. The column has a silver coated glass outer-shell and its evacuated annulus is sealed to prevent heat losses. The distillation pot was a 2000 ml 3-neck flask, with a thermowell reaching down to its bottom. A heating mantel with a circumvential zipper jacket snugly covered the 3-neck flask. This heating mantel, was covered with glass wool to help prevent heat losses from the apparatus. The liquid splitter was an electromagnetic type. A 500 ml graduated jacketed receiver was used to collect the sample. The receiving line and the stop-cock on the bottom of the receiver were wrapped with heating tape to prevent material from solidifying at those points.

C. Carbolic Oil Distillation Procedures

A 3-neck distillation flask was weighed to obtain tare weight. The sample was then placed in the flask and weighed on a beam type balance. This was the only weight that was not done on the Mettler balance. This weight is accurate to ±1 gram. Boiling chips were put in and weighed. The weight was subtracted out of the final material that was left in the bottom of the pot. The 3-neck flask was then connected to the distillation column and the vacuum pump was turned on to have an absolute pressure of 100 mm Hg at the top of column and receiver. The column was then heated under total reflux until equilibrium was established. At this point, the reflux ratio was then set at 20 to 1. Samples were taken off at approximately 5%, 10%, 15%, 20%, 25% and 5% from thereafter. When the sample was taken, the barometer was checked from time to time and the vacuum was reset when needed for maintaining the overhead pressure at 100 Torr. The pot and the overhead temperatures were recorded.

After each sample was taken, it was set to cool down. After cooling, the sample was weighed in a tarred receiver. The data are shown in Table II.

D. Light Creosote Oil Distillation Procedures

The light creosote oil was done in two separate distillations. The same procedures were followed as in preparing the sample, weighing and setting up the pressure. In the first distillation, a primary crude fractionation of the creosote oil was performed. There were five cuts in all. The reflux ratio of this first distillation was 5 to 1. The original sample weight was 1200 gm. Cut I ranged from 30°C to 200°C. Cut Number 2 was from 200°C to 250°C. Cut Number 3 was from 250°C to 280°C. Cut Number 4 was 280°C to 315°C and Cut Number 5 was from 315°C to 345°C. The residue from this distillation was 121.8 grams. The samples from each of these primary crude fractionations were weighed and a total of 1054 grams of refined light creosote oil was placed in the distillation pot flask for the secondary fraction.

The second distillation was performed similarly to that of the carbolic oil residue. Temperatures, pressures and procedures for weighing the samples were the same. Different procedures were followed when the temperature in the pot became too hot during the second distillation of the refined light creoste cut. The pressure had to be reduced first to 70 mm Hg and later to 40 mm Hg to maintain the pot's temperature below 315°C and, thus, to prevent cracking of the hydrocarbons. The data are shown in Tables X and XI.

E. Measurement of Densities

The Detroit tar plant provided the density at low temperatures with each of the samples. The density of each sample was measured again at 60°F with a 25 ml picnometer. The results are summarized below:

STOCK	MEASURED SP. GR. T/20°F			
	Allied		This Work	
	60°F	293°F	60°F	295°F
Carbolic Oil	1.035	0.936	1.034	0.935
	100°F	267°F	100°F	265°F
Light Creosote Oil	1.103	1.036	1.1031	1.036

F. Qualitative Analyses

Each sample was submitted for infrared analyses. The infrared analysis of the distillation cuts were performed in standard equipment. A Beckman Model 12 spectrophotometer with an analytical range of 4,000 to 200 reciprocal centimeters was used in all analyses.

The sample was dissolved in Carbon Disulfide, placed in a 0.1 centimeter cell with Potassium Bromide windows and scanned under normal resolution conditions. Reference spectra were taken from the Sudtler Standard Reference collection, and assignments made where possible.

G. Vapor Pressure Measurements

All vapor pressure measurements were done in a glass cell, shown schematically in Figure 26. Due to the apparent limitation imposed by the nature of this apparatus, the data taken in this study were within the range of 2 to 800 Torr. The procedure was as follows.

Once major compounds were identified, cuts with similar major components were combined. The samples that were to be combined were heated until they became liquid and placed in a vapor pressure apparatus. Two constant temperature baths were used; one for heating and one for cooling. The constant temperature bath for the heating had silicon oil in the reboiler and the constant temperature bath for the cooling system had Dowtherm A or silicon oil when higher temperature ranges above 200°C were needed.

After the fraction was put into the apparatus, the pressure was set by cracking the bleed valve in vacuum system, and the levels of the mercury in the manometer were read with a catheometer. Each absolute pressure was determined by subtracting the difference from the barometric reading. At each experimental run, the sample was kept at equilibrium for approximately 60 minutes before the reading was taken, also, at 15 minute intervals, the barometer was read to make sure that the actual atmospheric pressure was recorded. If the reading did change, it was so noted and the vacuum adjusted. The apparatus was insulated with glass wool to prevent heat loss.

The results are shown in Tables I and IX.

H. Molecular Weight Measurement

Molecular weights were determined with a vapor pressure osmometer at Allied Chemical CRL Laboratories. Samples were submitted and the molecular weight of each raw sample was determined. The results are given in Tables II and X.

IV. ANALYTICAL WORK

A. Objective

The purpose of this part of the research was to identify the components present in the distilled cuts of the carbolic oil residue and the light creosote oil. Knowledge of the compounds and their nature provided information for understanding the differences between the experimental vapor pressures and predictions by the method of Maxwell-Bonnell (18 and 19)

B. Procedures

1. Qualitative Infrared Spectrophotometry

Thirty-four fractions were submitted for qualitative infrared analysis. A portion of each sample was dissolved in carbon disulfide. The spectra were recorded from 2 to 15 microns against a carbon disulfide reference spectrum with a Beckman Model 12 infrared spectrophotometer equipped with grating type dispersion optics. Reference compounds which are soluble in carbon disulfide were recorded in a like manner. The carbon disulfide insoluble compounds were blended with potassium bromide and then pressed into 1/2-inch diameter disks.

Twenty-six compounds were identified in the fractions as shown in Table III, XII. Some fractions could not be identified completely. In some instances, the spectra of the unidentified portions of the fractions suggested structures for which no reference spectra or samples are available.

Comparison of the spectra of the selected fractions with those of the available pure compounds indicated a lack of spectra necessary for a complete qualitative identification of blended creosote compounds. A list of the available reference compounds which boil between 173 and 450°C was used although at least 20 additional known coal tar components (or their spectra) in that boiling range were not available at this time.

2. Semi-Quantitative Infrared Spectrophotometry

The semi-quantitative method was devised after the qualitative infrared analyses were completed so that all of the major components could be included in the matrices. Some fractions were not completely identified (see qualitative analysis section) and in such cases, the methods give maximum concentrations due to the extraneous absorbances of unknown compounds. The amount of unidentified components in these cases were estimated by the differences between the sum of the known compounds and 100 per cent.

C. Results of the Spectrotometry Analyses

The accuracy of the analyses when one component was major (25%) and the measured absorbance was of the same magnitude as that obtained in the calibration, is estimated to be approximately ±10%. Complex mixtures such as encountered in the front end, intermediate fractions, and tail end fractions are probably not as accurate.

V. MEASUREMENT OF VAPOR PRESSURES AND PRESENTATION OF DATA OF COAL OILS

A. Experimental Measurements of Vapor Pressure Data

A study of mixtures requires a revision of our conception of vapor-pressure. Every material, by virtue of the movement of molecules within it, exerts a tendency to vaporize, even though it is far below its boiling point. In the case of a single compound, the tendency to vaporize or to project molecules into the surroundsings grows as the temperature is raised. When the internal pressure is equal to the pressure of the system, the material boils. At temperatures above the normal boiling-point, the vapor-pressure is greater than one atmosphere.

The vapor-pressure of a mixture is usually defined as the pressure exerted by the material when no vaporization occurs. If vaporization occurs, the composition of the material is no longer the same. The vapor-pressure of a mixture is a summation of its components. And if the system is ideally mixed, it obeys Raoult's law.

A simple method for measuring the vapor pressure was used in this study. The samples where contained in a vapor-pressure apparatus (Figures 26 and 28) and connected with a mercury manometer and a vacuum pump, a manostat and other auxiliaries.

Since the sample cell of the apparatus is surrounded by the heating medium, it could be assumed that the temperature in the entire cell was uniform. Also since the system is evacuated through a condenser, the error which could be produced by the presence of air or other permanent gases which have been dissolved, in the liquid or trapped by the mercury is avoided. The sample under vacuum reaches equilibrium and is rendered free of gases in a relatively short time. Hence, each point was maintained at a temperature and pressure for sixty minutes. This provided an adequate time to purge out any non-condensible gases (i.e. air) and reduce that source of error.

B. Results of The Distillation of Carbolic Oil Residue

The results of the distillations for the carbolic oil residue can be found listed in Table II. The equipment set up can be found on Figure 27.

The carbolic oil residue was distillable over a range of temperatures from 209.3°C to 289.4°C and 100mm Hg. Since the temperature was not near the cracking point, the vacuum had to be adjusted only for slight changes. A total of fifteen cuts were obtained. 97.07% of the original sample was distilled and only 8.72 gm or 0.85% was listed.

The carbolic oil residue distillate material is composed mainly of Naphthalene, methylnaphthalene, and Di and Tri Methyl Naphthalene, together with lesser amounts of anthracene, phenanthrene and fluorene. See Table III.

C. Vapor Pressure Measurements on The COR Cuts

Vapor pressure measurements were performed on five narrow boiling cuts. Results are shown in Table I. Cut 1 ΔT was 19°C, Cut 2 ΔT was 10°C, Cut 3 ΔT was 15.5°C, Cut 4 ΔT was 17.4°C and Cut 5 ΔT was 77°C. One must realize that although Cut 5 ΔT was 77°C, the major components in this fraction were higher boiling aromatics, i.e. phenanthrene, fluorene and anthracene.

A painstaking effort was given to monitoring changes in temperature or barometric conditions and adjusting the vacuum. Accordingly so, the experimental results obtained in this work do represent steady state conditions. The meaningful representation of the experimental results would not be possible if the steady state conditions were not obtained.

The attainment of steady state in the apparatus at the conditions of operations is supported by the following:

1. Following observation of steady state incipient distillation/condensation, the temperature and pressure were checked at 15 minute intervals. Once no changes in temperature and pressure occurred, an initial reading was taken.
2. Once the initial reading was taken, it was checked and confirmed at 10 minute intervals.

3. The apparatus was wrapped in glass wool after heatup and kept in a lab hood with heater lights to prevent heat losses to the atmosphere.
4. Heating and cooling baths were kept at constant temperatures and were monitored at the same frequency as was the sample.

It is felt that with the above steps taken, the apparatus' operation at steady state was confirmed for each run.

Figures 11 to 15 illustrate the data which are listed in Tables IV and VIII and show a consistency for points falling on the vapor pressure curve. Figure 24 illustrates each of the vapor pressure curve as a function of log P in mm Hg versus 1/T°K. This plot also indicates very little scatter of data.

D. Results of The Distillation on This Light Creosote Oil

The data of the distillation of the light creosote oil are given in Table X. The equipment set-up was the same as that used in the carbolic oil residue distillation. A sample of 1200 grams was placed in the distillation pot and 5 major cuts were removed. Temperature ranges for the cuts are as follows: Cut 1 0 - 200°C; Cut 2 200 - 250°C; Cut 3 250 - 280°C; Cut 4 280 - 315°C, Cut 5 315 - 345°C.

A total of 88.71% or 1064.3 grams of refined creosote oil was obtained. The residue and holdup material in the column were discarded.

A sample of 1054 grams of refined creosote oil was placed in the same distillation set up once the apparati have been dismantled and cleaned.

The LCOR was distilled over a range of temperatures from 146°C to 291°C and a pressure range of 100mm Hg to 40mm Hg. Results are listed in Table XI. During collection of fraction 18, the temperature in the distillation pot became too high, i.e. it exceeded 315°C, whenever that happened, pressure was reduced and the apparatus was cooled down to 300°C. The above procedure had to be repeated when fraction 19 was collected, 90.1% of the original sample or 949.6 grams of the

LCOR was distilled. The residue when cooled appeared like a black solid coal tar bottoms and resembled pitch. This residue and the charred distillation pot were discarded.
For a detailed compositional breakdown of the LCOR, see Table XII.

Two problems were encountered during the distillation. When Cut 13 was being collected, the tube leading the condensate from the liquid splitter to the receiver broke and, also, the pressure dropped as low as 97.4mm Hg on Cut 13.

E. Vapor Pressure Measurement on The LCOR Cuts

Vapor pressure measurements were performed on 8 cuts. Results are shown in Table IX. The boiling ΔT ranges are listed as follows:

Cut 1 ΔT was 22.6°C; Cut 2 ΔT was 32.7°C; Cut 3 ΔT was 14.6°C; Cut 4 ΔT was 8.3°C; Cut 5 ΔT was 25.1°C; Cut 6 ΔT was 7.7°C, Cut 7 ΔT was 14.4°C, Cut 8 ΔT cannot be determined. Figures 16 - 22 illustrate the experimental data and again show a consistency for points falling on the vapor pressure curve. Very little scatter of the data was noted on any of the vapor pressure curves.

Figure 23, on the other hand, illustrates the need for knowing the boiling point at 760mm Hg. Since this data point is not always taken due to the possibility of cracking, it is the experimenter's or designer's best guess as the appropriate place for a given curve on this Figure.

Figure 25 illustrates the group of curves that seem to be straight lines of vapor pressure-temperature data of the light creosote oil stock fractions. Curves six and seven have no point at 20mm Hg due to solids in the condenser.

The temperatures at which Cuts Number 17 through 19, shown as Curve 8, boils under the pressure 600 and 760mm Hg could not be measured due to concern over cracking. Therefore, the information gathered on this cut that is shown in Table XX and as Curve 8 of Figure 25 illustrate only lower pressure data which were taken at temperatures below 315°C.

The accuracy of measurements of vapor pressures of cuts of the carbolic oil residue should be considred high. This is because the distillation was carried out until the distillation pot was dry. The light creosote oil was refined first and a portion of the oil was discarded. This fraction contained very high boiling point material and was outside the range of interest. A small amount of materials from each cut was left in the sample bottle. This should not have introduced any errors into the data since the liquid that was collected in the sample bottles was homogenous. The major sources of errors could be reading temperatures, pressures and infrared analyses, though extreme care was used in recording temperature and pressures.

VI. CORRELATION OF THE VAPOR PRESSURE DATA

A. Evaluation of The Vapor Pressure Data

Vapor pressure data are useful for engineering work when suitably correlated in the form of pressure versus temperature graphs. The correlations are needed to describe the equilbrium in real systems of interest which may contain a large number of components of various natures in wide ranges of compositions, (i.e. like those in the coal tar oils.) In addition, the temperature and pressure can vary over wide ranges. The possible combinations of variables of interest is so large that it is impractical to attempt direct experimental observation on all of them and the limited quantity of experimental data must be generalized through the development of correlations. Thus the ultimate usefulness of the data reported here will depend on their test of the Maxwell-Bonnell correlation. In the following sections, I will discuss the testing in two ways: the test of existing correlations and the recommendation for development of new correlations with the data. The accuracy of existing correlations can be determined when tested with experimental data. The results will indicate to the engineer the need to use correction factors if necessary and when systematic deviations are uncovered. Any need for the development of new correlations will also become obvious.

The vapor pressure data which are illustrated in Figures 11 - 25 indicate good agreement with very little scatter. Figures 24 and 25 show a graphical presentation of log P versus 1/T. This plot of log P versus 1/T should be linear and this is borne out by the data. Although one must realize over a wide temperature range there are significant deviations from linearity because some of the approximations made in the devaition of the Clausius Clapeyron Equation.

Curves 6 and 7 on Figure 29 are missing the 20mm Hg point due to solids in the condenser and curve 8 is missing the 760mm Hg and 600mm Hg points due to a high temperture in the vapor pressure still.

B. Computer Runs and Comparisons of Calculated Values Versus New Data

1. Procedure

Each set of experimental data was run on the computer program with the Maxwell-Bonnell corrleation. The results of the computer runs can be found in Appendix 3. Also a listing of the computer programs that were used is in Appendix 3.

Comparison of the new experimental data with the Maxwell-Bonnell correlation indicates large deviations as can be found in Figures 9 and 10. This test case indicates two things: one is that T correlation for the individual points is only a stop gap measure for correcting the effect of noncompliance and, two, coal oil requires another pivot point.

2. Tabulating and Plotting ΔT Values for Individual Points

The study described herein had its initiation in computations related to simulating recovery of anthracene from coal tar oil. A comparison was made between values of vapor pressure of anthracene, phenanthrene and carbazole predicted by the method of Maxwell-Bonnell (M-B) and values from the literature. The comparison indicated that if the M-B procedure were to be used for predicting the low range vapor pressure of phenanthrene, with UOPK=9.2, the constant of Equation (No.3), the mathematical expression for the lines in Figure 5, should be changed from 2.5 to 6.69. Even with this change, vapor pressures could not be predicted with reliability.

The above stop-gap measure was adequate for the purpose. However, it was recognized that the substitute coefficient would not serve in predicting pressures above one atmosphere.

A distilled sample of SRC-II, which had been used by Prof. Tarrer at Auburn University in studying solubility of hydrogen, and samples of two coal tar oils, one, the coal tar "anthracene oil", the feed stock for recovering anthracene and carbazole, and, two, a sample of carbolic oil residue was used. The TBP curves of these three distillations are shown in Figures 3, 7 and 8. Many fractions that were obtained were further studied.

Vapor pressure data were analyzed, each to evaluate a value of ΔT that would be required, to correct for the effect of noncompliance with the M-B procedure for paraffins (UOPK=12). The results, some are shown on Figure 9 led to the following, preliminary observations:

a. With reference made to Figure 9 even in the portions of the curves of ΔT vs. measured P_i that are almost straight lines, the lines do not fall where Equation 3 would predict. Indeed the discrepancies are significant.

b. For any pure compound or a fraction with K-10 the boiling point corrections ΔT do not plot as a straight line, as suggested in Figure 5.

c. Values of ΔT calculated from experimental data taken at temperatures above the boiling points indicate a tendency toward very sharp declines, suggesting unrealistic, and probably unreliable extrapolations to vapor pressures higher than 10 atmospheres.

3. New Coal Oils Require Another Correlation Pivot Point

Observations indicated that the correlation of vapor pressures of aromatic compounds and fractions with n-hexane being the reference compound, the lines tend to converge at a pivot point which is different from the one selected by Maxwell and Bonnell for paraffinic stocks. (See Figure 10).

The data presented herein, when plotted on Maxwell-Bonnell charts indicated that coal oil fractions have slopes that are different from those of the paraffins that have the same boiling points, the third parameter lines of Figure 5 etc. Also, some of the fractions that were studied did not conform to the general tendency of their brethern to converge when plotted as lines on the

M-B charts. Those nonconforming fractions, when analyzed, were found to contain up to 20% of oxygenated compounds, e. g. dibenzofuran and diphenyl oxide.

VII. SUMMARY, CONCLUSION AND RECOMMENDATIONS

A. Summary

Experimental data were taken and were used to test the Maxwell-Bonnell correlation. The original correlation was found to give large systematic deviations at the conditions of temperature and pressures of interest. Review of the nature of the deviations led to the conclusion that the basic scheme of the Maxwell Bonnell correlation can be used but should be modified for describing the behavior of coal tar oils. A proposed correlation was worked out as part of this study.

B. Proposed Modifications For The Maxwell Bonnell Correlation

1. General Statement

The Maxwell-Bonnell equation exhibits weaknesses when used for predicting vapor pressure of some coal tar oil fractions. Some of the major causes for this weakness are:

a. The basis used in the development of the Maxwell-Bonnell equation was n-hexane.Since coal tar oils are much more aromatic, these properties greatly affect the vapor pressure of a pseudo component mixture. Hence, the Maxwell-Bonnell equation is not able to properly predict the vapor pressure due to the above mentioned fact.

b. Another weakness in the equation is that it was not developed for bonded compounds that have oxygen in them, i.e. dibenzofuran and diphenyl oxide.

The larger deviations that were observed indicate that a new empirical correlation is needed. A modified Maxwell-Bonnell type should be developed for predicting vapor pressures of aromatic compounds and liquid fractions derived from coal tar. It should be applicable for predicting vapor pressures of coal tar oil characterized by UPOK values between 8 and 11.

2. Need For Data in Wider Temperature Ranges

The need for data in a wider temperature range is a necessity. Since the data in this work were taken within a narrow range, they could not provide sufficient information for developing a new or modified correlation.

3. Combining The Data From This Study With Others

A sufficient amount of information, could be gathered from combining the data from this work with other data, such as those from Exxon (13), Gulf (27) and vapor pressures of pure compounds (1, 2, 3, 4).

4. Better Reference Compound is Needed

Since the basis for development for the Maxwell-Bonnell equation was n-hexane, the new correlation could be developed using a new reference compound such as naphthalene and one that is more aromatic in nature.

APPENDIX 1

Table I

VAPOR PRESSURES OF CARBOLIC OIL RESIDUE FRACTIONS

PRESSURE	FRACTION 1 - 2	FRACTION 3 - 5	FRACTION 6 - 8	FRACTION 9 - 11	FRACTION 12 - 15
mmHG	Temp °C	Temp °C	Temp °C	Temp °C	Temp °C
760*	215.5	251.6	262.5	282.5	340.6
600	205.5	241.5	251.1	271.4	328.3
500	198.6	234.4	243.4	261.1	318.8
400	190.2	227.2	233.8	250.5	308.5
300	179.8	215.5	221.6	237.7	293.7
200	167.7	193.8	207.7	223.3	274.0
100	147.7	171.7	182.2	196.6	249.2
50	120.5	153.8	161.6	175.1	223.1
20	102.2	129.4	136.1	147.7	Solids in Condensor

*For the exact pressure, see each individual table (IV - VIII)

Table II
CARBOLIC OIL RESIDUE DISTILLATION

Column	1" 20 plate Oldshaw	Density	
Pressure	100 mm Hg	60°F	1.035
R/R	20/1	293°F	.936

Molecular Weight = 127

Material Balance	Sample weight	1020 gm
	Distillate Fraction	990.15 gm
	Contents of Vacuum Trap	9.73 gm
	Residue and Holdup	11.40 gm
	Overall Loss	8.72 gm

Fraction	Pressure mm Hg	Pot Temp. ° C	O H Temp. ° C	Wt/Fract. gm	Accum wt gm	Wt. %
1	100.0	209.3	140.5	60.38	60.38	5.9
2	100.0	212.2	159.5	56.74	117.12	11.48
3	100.1	221.0	164.4	111.80	228.98	22.45
*4	99.8	228.7	168.1	70.84	299.82	29.39
5	100.3	234.5	174.4	56.94	356.76	34.97
6	100.1	241.5	179.6	59.10	415.76	40.76
7	100.0	248.3	184.4	52.96	468.72	45.95
8	99.9	255.2	189.9	54.22	522.94	51.26
*9	99.9	262.5	194.6	65.24	588.18	57.66
10	100.1	271.2	200.4	67.54	655.72	64.28
11	100.0	278.2	207.3	64.70	720.42	70.62
*12	100.0	285.0	214.8	661.0	786.52	77.11

Fraction	Pressure mm Hg	Pot Temp. °C	O H Temp. °C	Wt/Fract. gm	Accum. Wt. gm	Wt. %
13	100.0	288.3	247.4	65.71	852.23	83.55
*14	100.1	289.4	269.4	65.30	917.53	89.95
15	99.9	289.4	284.3	72.62	990.15*	97.07

*Pot Dry

*By fraction number denotes shutdowns

Table III

CARBOLIC OIL RESIDUE
INFRARED SPECTROPHOTOMETRY ANALYSIS OF MAJOR COMPONENTS

Fraction Number	Wt%	Component
1-2	15.4	3-5 Dimethyl coumarone
	53.8	Naphthalene
	9.6	Thianaphthalene
	5.3	2 Methyl Naphthalene
	15.9	Unknowns
3-4-5	27.8	2 Methyl Naphthalene
	32.6	1 Methyl Naphthalene
	18.5	2 Ethyl Naphthalene
	7.2	Bi Phenyl
	13.9	Unknowns
6-7-8	11.1	2-6 Di Methyl Naphthalene
	15.7	1-3 Di Methyl Naphthalene
	22.7	1-7 Di Methyl Naphthalene
	27.3	1-6 Di Methyl Naphthalene
	8.6	1-5 Di Methyl Naphthalene
	14.6	Unknowns
9-10-11	11.3	1-5 Di Methyl Naphthalene
	9.6	Acenaphthalene
	16.7	Di Benzil
	24.7	2-3-5 Tri Methyl Naphthalene
	23.8	2-3-6 Tri Methyl Naphthalene
	13.9	Unknowns
12-15	11.8	Fluorene
	22.6	Anthracene
	62.4	Phenanthrene
	3.2	Unknowns

Table IV

VAPOR PRESSURE OF
CARBOLIC OIL RESIDUE
Fraction 1-2

mmHg	Temp °C	1/T°K X 10-3
758.8	215.5	2.05
600	205.5	2.09
500	198.6	2.12
400	190.2	2.16
300	179.8	2.21
200	167.7	2.27
100	147.7	2.38
50	120.5	2.54
20	102.2	2.66

Table V

VAPOR PRESSURE OF CARBOLIC OIL RESIDUE
Fraction 3-4-5

mmHg	Temp °C	1/T°K X 10 - 3
754.2	251.6	1.91
600	241.5	1.94
500	234.4	1.97
400	227.2	2.00
300	215.5	2.05
200	193.8	2.14
100	171.7	2.25
50	153.8	2.34
20	129.4	2.48

Table VI

VAPOR PRESSURE OF
CARBOLIC OIL RESIDUE
Fraction 6-7-8

mmHg	Temp °C	1/T°K X 10 - 3
755.6	262.5	1.87
600	251.1	1.91
500	243.4	1.94
400	233.8	1.97
300	221.6	2.02
200	207.7	2.08
100	182.2	2.20
50	161.6	2.30
20	136.1	2.44

Table VII

VAPOR PRESSURE OF CARBOLIC OIL RESIDUE

Fraction 9-10-11

mmHg	Temp ^{o}C	$1/T^{o}K \times 10 - 3$
756.0	282.5	1.80
600	271.4	1.84
500	261.1	1.87
400	250.5	1.91
300	237.7	1.96
200	223.3	2.01
100	196.6	2.13
50	175.1	2.23
20	147.7	2.38

Table VIII

VAPOR PRESSURE OF CARBOLIC OIL RESIDUE
Fraction 12-15

mmHg	Temp °C	1/T°K X 10 - 3
757.1	340.6	1.63
600	328.3	1.66
500	318.8	1.69
400	308.5	1.72
300	293.7	1.76
200	274.0	1.83
100	249.2	1.91
50	223.1	2.02
20		Solidifying in condenser

Table IX

VAPOR PRESSURE
OF
LIGHT CREOSOTE OIL REFINED FRACTIONS

PRESSURE mmHg	FRACTION 1 - 2 Temp °C	FRACTION 3 - 4 Temp °C	FRACTION 5 - 6 Temp °C	FRACTION 7 - 8 Temp °C	FRACTION 9 - 10 Temp °C	FRACTION 11 - 14 Temp °C	FRACTION 15 - 16 Temp °C	FRACTION 17 - 19 Temp °C
760*	226.6	272.2	284.7	296.4	322.7	342.3	357.8	Not Taken
600	217.6	261.3	272.6	289.1	312.2	329.4	349.2	Not Taken
500	208.8	254.9	263.4	282.1	302.0	320.0	334.3	359.3
400	200.5	249.4	251.2	272.2	288.7	310.1	323.6	346.1
300	188.3	235.2	239.1	260.2	274.2	294.9	308.1	329.3
200	174.4	218.7	226.7	244.4	258.6	275.8	288.3	310.2
100	152.3	193.4	206.7	220.9	241.7	253.4	267.4	283.7
50	131.6	171.1	183.6	194.7	217.8	227.8	241.3	260.3
20	107.7	146.8	159.9	171.8	196.4	Solids in Condenser	Not Taken	230.7

*FOR EXACT PRESSURE, SEE TABLES (XIII - XX)

Table X

CRUDE DISTILLATION OF CREOSOTE

Column 1" 20 Plate Oldshaw R/R = 5/1

Pressure 100 mm Hg

Cuts	1	0 - 200°C
	2	200 - 250°C
MW = 160	3	250 - 280
	4	280 - 315
	5	315 - 345

Material Balance

Sample Wt.	1200 gm
Distillation Fraction	1064.3gm
Vacuum Trap	7.4gm
Residue	121.8gm
Loss	6.5gm

Density

1.103 @ 100° F

1.036 @ 267° F

Fraction	OH	POT	PRESS MM Hg	ACCUM Wt. %
1	200	251	100	12.1
2	250	286	100	39.32
3	280	304	100	64.53
4	315	335	100	73.96
5	345	368	100	88.71

Total Weight of Refined Creosote Oil 1054 gm

Loss of 10.3 g for Transfer

Table XI

REFINED DISTILLATION OF CREOSOTE

LCO - LIGHT CREOSOTE OIL FROM DETROIT

R/R 20/1

Wt. of Sample 1054gm

Column 1" 20 Plate Oldshaw

Density	100°F	1.103
	267°F	1.036

Wt. of Sample	1054 gm
Distillate	949.6gm
Residue	94.75gm
Trap	6.32
Loss	3.28gm

FRACTION	PRESSURE mm Hg	O H TEMP °C	BOTTOM TEMP. °C	WT OF SAMPLE gm	WT ACM gm	% WT ACCUM	
1	100.0	146.6	180.2	44.26	44.26	4.2	
2	99.9	169.2	211.0	49.53	93.80	8.9	
3	100.1	197.1	214.8	41.11	134.91	12.8	
4	100.0	201.9	218.0	47.43	182.34	17.3	
*5	100.0	206.3	222.7	52.70	235.04	22.3	Broken Line Receiver
6	99.9	216.5	227.1	48.48	283.52	26.9	
7	100.0	219.6	234.3	41.11	324.63	30.8	
8	100.0	224.8	245.7	49.54	374.17	35.5	
*9	99.8	238.4	253.4	53.75	427.92	40.6	
10	100.0	249.9	257.0	47.43	75.35	45.1	
11	100.0	252.0	258.6	59.02	534.37	50.7	
12	100.0	252.1	258.9	49.54	583.91	55.4	
13	99.9	253.8	268.1	56.92	640.83	60.8	Pressure to 97.4
14	100.1	257.6	275.4	51.64	692.47	65.7	
15	100.0	265.9	319.2	53.76	746.23	70.8	

Table XI (cont'd)

FRACTION	PRESSURE mm Hg	O H TEMP °C	BOTTOM TEMP. °C	WT OF SAMPLES gm	WT ACM gm	WT.% ACCUM.
*16	100.0	272.0	322.6	51.64	797.87	75.7
17	100.0	291	335.3	54.81	852.68	80.9
18	1* 70	276.1	328.9	52.70	905.38	85.9
19	2* 40	252.9	348.	44.27	949.65	90.1

*By Fraction Numbers denotes shutdowns

1*Temperature in pot becomes too high compounds might crack reduced pressure.

2*Same as 1.

Table XII

LIGHT CREOSOTE OIL
(ANTHRACENE OIL)
INFRARED SPECTROPHOTOMETRY ANALYSIS
OF MAJOR COMPONENTS

Fraction Number	Wt%	Components
1-2	43.7	Naphthalene
	20.8	Thianaphthene
	15.4	2 Methylnaphthalene
	11.0	Quinoline
	9.1	Unknowns
3-4	23.2	2 Methylnaphthalene
	20.9	1 Methylnaphthalene
	18.7	Acenaphthylene
	10.3	2-3 Di Methylnaphthalene
	6.4	1-6 Di Methylnaphthalene
	3.2	Dibenzofuran
	17.3	Unknown
5-6	9.8	Acenaphthylene
	18.7	Dibenzofuran
	57.8	Fluorene
	13.7	Unknowns
7-8	7.5	Dibenzofuran
	33.6	Fluorene
	46.8	3 Methydiphenylene Oxide
	12.1	Unknown
9-10	12.8	3 Methydiphenylene Oxide
	29.3	9-10 Dihydro Anthracene
	47.6	Phenanthrene
	10.3	Unknowns

Table XII (cont'd)

Light Creosote Oil

Fraction Number	Wt%	Components
11-12-13-14	33.6	Phenanthrene
	29.7	Anthracene
	18.7	3 Methylphenanthrene
	7.9	Carbazole
	10.1	Unknown
15-16	9.3	3 Methylphenanthrene
	36.7	Carbazole
	27.8	4-5 Methylphenanthrene
	10.6	9 Methylanthracene
	15.6	Unknown
17-18-19	9.1	9 Methylanthracene
	13.4	2 Methylcarbazole
	24.7	Fluoranthene
	27.8	Pyrene
	24.4	Unknown

Table XIII

VAPOR PRESSURE OF LIGHT CREOSOTE OIL REFINED

Fraction 1-2

mmHg	Temp °C	1/T°K X 10 - 3
758.4	226.6	2.00
600	217.6	2.04
500	208.8	2.07
400	200.5	2.11
300	188.3	2.17
200	174.4	2.23
100	152.3	2.35
50	131.6	2.47
20	107.7	2.63

Table XIV

VAPOR PRESSURE OF LIGHT CREOSOTE OIL REFINED

Fraction 3-4

mmHg	Temp °C	1/T°K X 10 - 3
758.3	272.2	1.83
600	261.3	1.87
500	254.9	1.89
400	249.4	1.91
300	235.2	1.97
200	218.7	2.03
100	193.4	2.14
50	171.1	2.25
20	146.8	2.38

Table XV

VAPOR PRESSURE OF LIGHT CREOSOTE OIL REFINED

Fraction 5-6

mmHg	Temp °C	1/T°K X 10 - 3
757.2	284.7	1.79
600	272.6	1.83
500	263.4	1.86
400	251.2	1.91
300	239.1	1.95
200	226.7	2.00
100	206.7	2.08
50	183.6	2.19
20	159.9	2.31

Table XVI

VAPOR PRESSURE OF LIGHT CREOSOTE OIL REFINED

Fraction 7-8

mmHg	Temp °C	1/T°K X 10 - 3
752.5	296.4	1.76
600	289.1	1.78
500	282.1	1.80
400	272.2	1.83
300	260.2	1.87
200	244.4	1.93
100	220.9	2.02
50	194.7	2.14
20	171.8	2.25

Table XVII

VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
Fraction 9-10

mmHg	Temp °C	1/T°K X 10 - 3
758.7	322.7	1.68
600	312.2	1.71
500	302.0	1.74
400	288.7	1.78
300	274.2	1.83
200	258.6	1.88
100	241.7	1.94
50	217.8	2.04
20	196.4	2.13

Table XVIII

VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
Fraction 11-14

mmHg	Temp °C	1/T°K X 10 - 3
757.8	342.3	1.62
600	329.4	1.66
500	320.0	1.69
400	310.1	1.71
300	294.9	1.76
200	275.8	1.82
100	253.4	1.90
50	227.8	2.00
20		Solids in Condenser

Table XIX

VAPOR PRESSURE OF LIGHT CREOSOTE OIL REFINED

Fraction 15-16

mmHg	Temp °C	1/T°K X 10 - 3	
758.1	357.8	1.58	
600	349.2	1.62	
500	334.3	1.65	
400	323.6	1.68	
300	308.1	1.72	
200	288.3	1.78	
100	267.4	1.85	
50	241.3	1.94	Some solids in condenser
20		Not Taken	

Table XX

VAPOR PRESSURE OF LIGHT CREOSOTE OIL REFINED

Fraction 17-18-19

mmHg	Temp ^{o}C	$1/T^{o}K \times 10 - 3$
755.4	1*	Not Taken
600	2*	Not Taken
500	359.3	1.58
400	346.1	1.61
300	329.3	1.66
200	310.2	1.71
100	283.7	1.78
50	260.3	1.87
20	230.7	1.98

*1 - *2 Due to equipment limitation last two points were not taken.

In addition chances of material cracking might be encountered.

Table XXI

SAMPLE OF SLOPES AND INTERCEPT

FRACTIONS	SLOPE, A	INTERCEPT, B
COR 1 + 2	1.50487	-0.0000818
COR 3 + 4 + 5	1.60205	-0.0000669
COR 6 - 8	1.63939	-0.0000749
COR 9 - 11	1.64443	-0.0000200
COR 12 - 15	1.86137	-0.0000594
LCO 1 + 2	1.50848	-0.0000493
LCO 3 - 4	1.69607	-0.0000949
LCO 5 - 6	1.85217	-0.0002303
LCO 7 - 8	1.86616	-0.0001827
LCO 9 - 10	2.07541	-0.0003224
LCO 11 - 14	1.94232	-0.0001313
LCO 15 - 16	1.98475	-0.0001243
LCO 17- 19	1.54444	-0.0002519

Table XXII

Δ T FOR LIGHT CREASOTE OIL FRACTIONS

FRACTIONS	Δ T at 0.1
1 - 2	+ 6
3 - 4	+ 3
5 - 6	+ 2
7 - 8	- 7
9 - 10	+19
11 - 14	+18
15 - 16	+22

Table XXIII

Vapor Pressure of SRC - II
Recycle Oil - Auburn Sample

Pressure MMHg	Temp. °C
758	218
400	200
300	184
205	170
100	154
50	138
20	106
6	81

Table XXIV

True Boiling Point (30/5) Distillation of
SRC Recycle Oil
Sample obtained from Auburn University

Vol % off	Overhead Pressure mmHg	Observed t°C	Atmospheric T_B	Sp. gr. 15/20	°API	Viscosity (cp)		Molecular Weight	
						@ 100°F	@ 210°F	Measured	Calc. (d)
Original Sample				1.035	5.2	4.968	1.397	150	
0.3	760 (a)	150		---					
5.0	760 (a)	188		0.9528	17.00				
12.0	760 (a)	202		0.9718	14.10				
18.6	760 (a)	212		0.9823	12.55				
25.	760 (a)	216		Solid					
31.6	760 (a)	225		Solid					
32.85	20	120	240 (c)	Solid	9.72	3.33	1.156	150	161
39.35	20	141	264 (c)	0.9935	10.92				
45.84	20	168	297 (c)	1.0198	7.24				
52.33	20	182	313.3 (c)	1.032	5.45				
58.83	20	219	356.11 (c)	1.0206	7.16				
65.32	20	241	381.67 (c)	1.0520	3.0				
70.77	20	261	407.7 (c)	1.0590	2.4				
77.27	0.6	161	---	Solid					
83.7	0.6	189	470.00 (c)	1.1040	- 3.33				
89.6	0.6	225	---	Solid					

Notes:
- (a) Adjusted
- (b) Measured at Allied Chemical's Laboratory.
- (c) Calculated, using the Maxwell Bonnell
- (d) Calculated, using the Winn Chart

DG:dh

APPENDIX 2

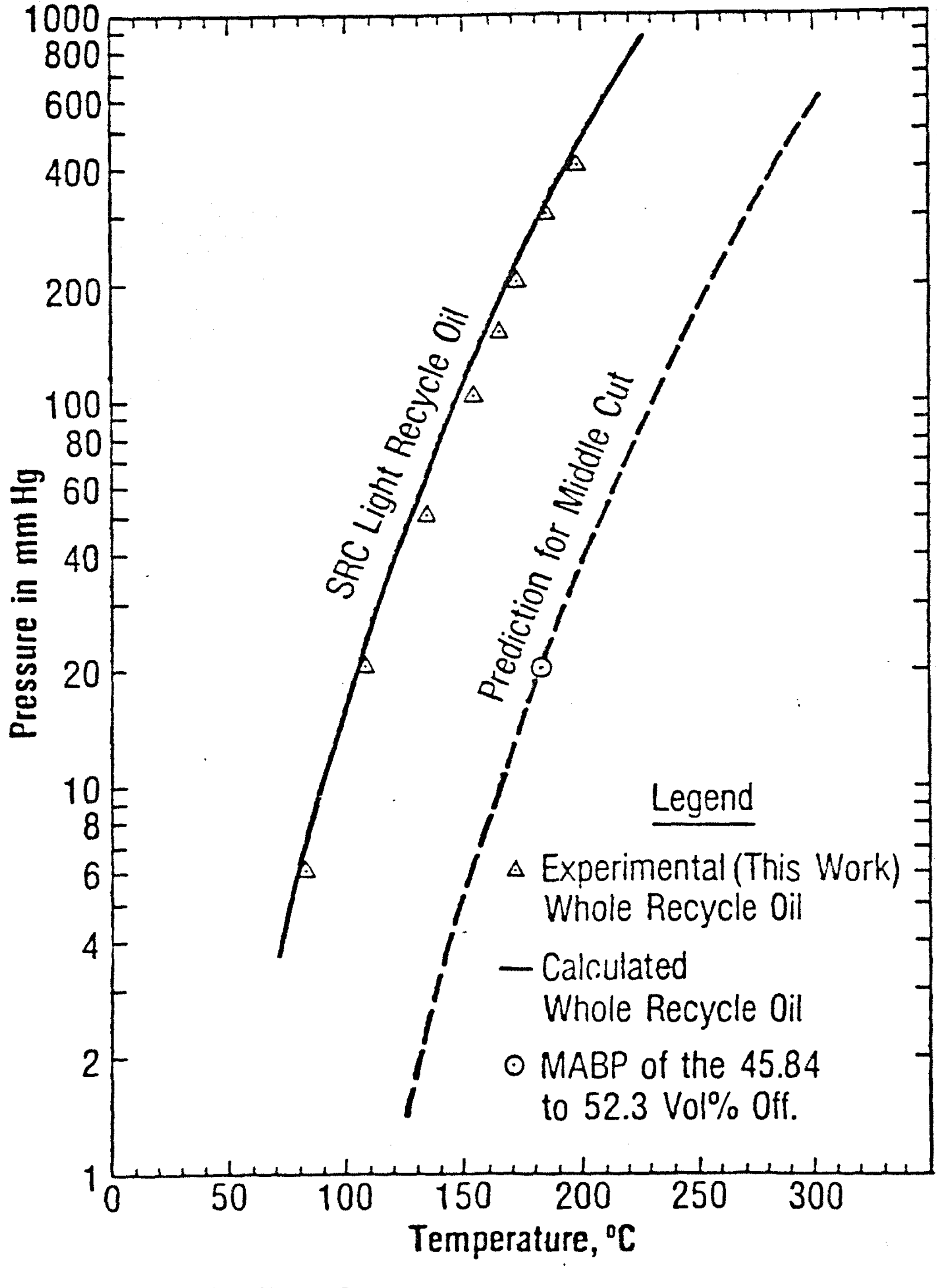


FIGURE 1. VAPOR PRESSURE OF SRC LIGHT RECYCLE OIL (OIL SAMPLE OBTAINED FROM PROF. TARRER, AUBURN UNIVERSITY).
Data from Table XXIII

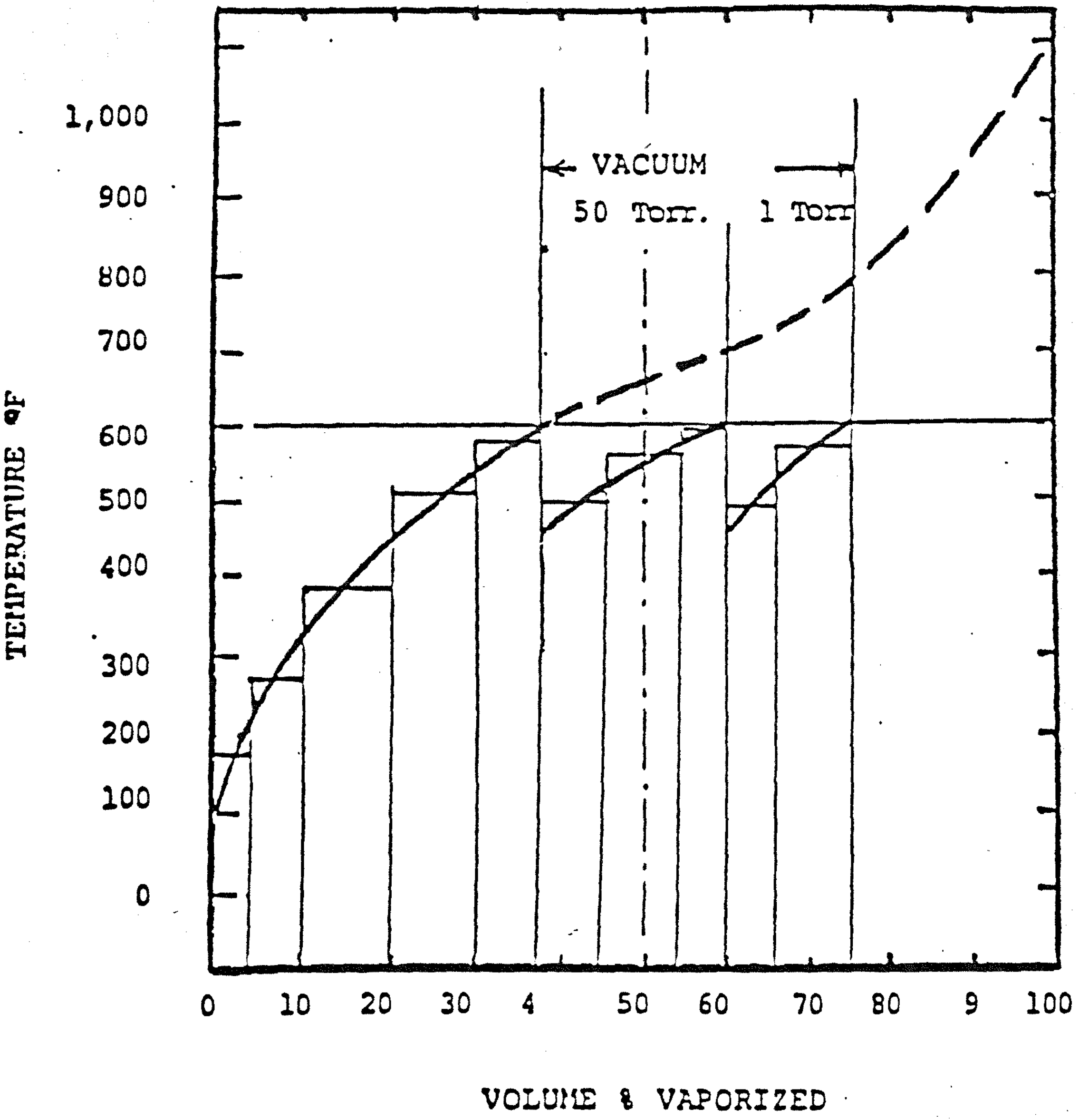


Figure 2. True Boiling Point Distillation and Interpretation of Data taken under vacuum.

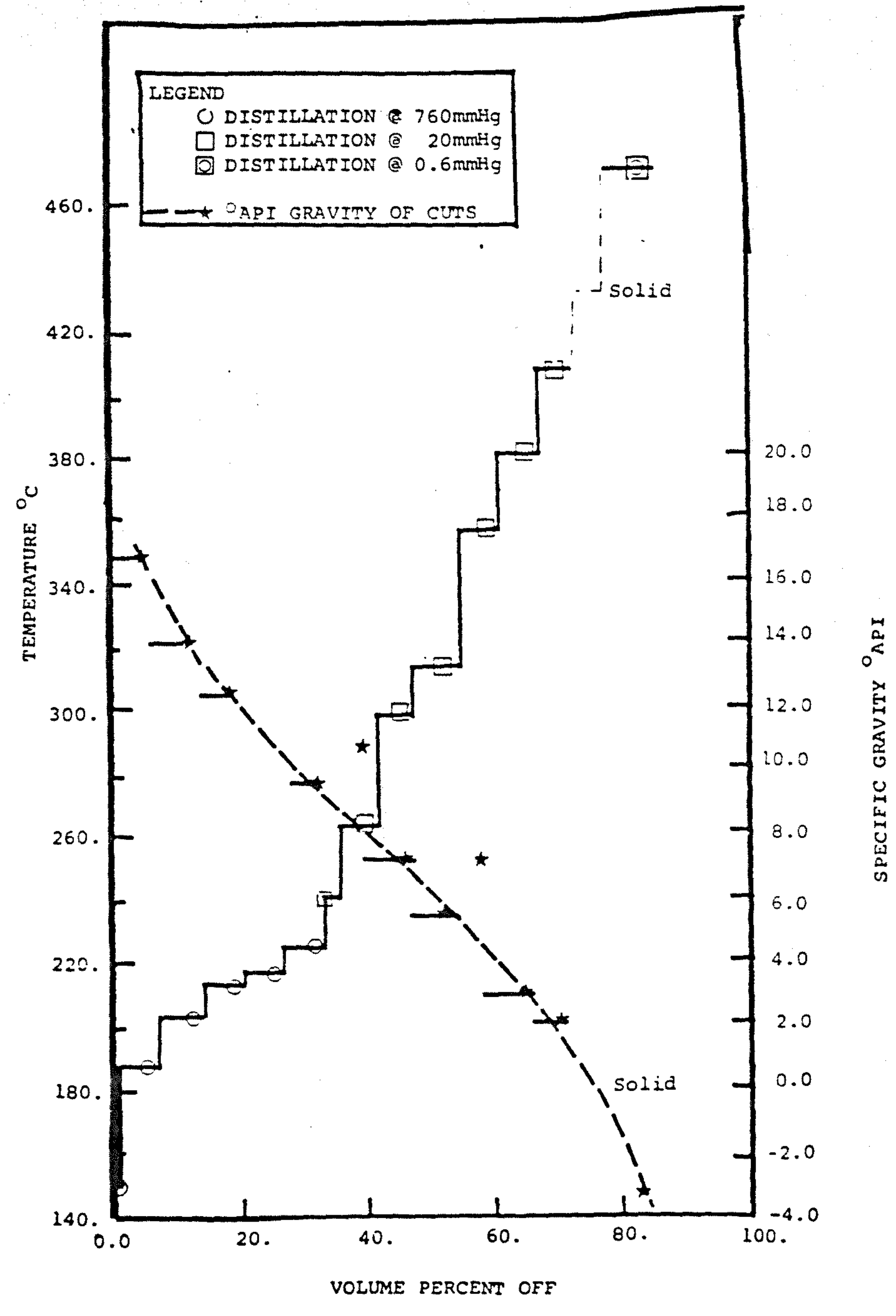


FIGURE 3. GRAVITY AND DISTILLATION CURVE FOR SRC RECYCLE OIL (SAMPLE OBTAINED FROM AUBURN UNIVERSITY), OLDERSHAW COLUMN 30 TRAYS; 5 TO 1 REFLUX RATIO.

Data from Table XXIV

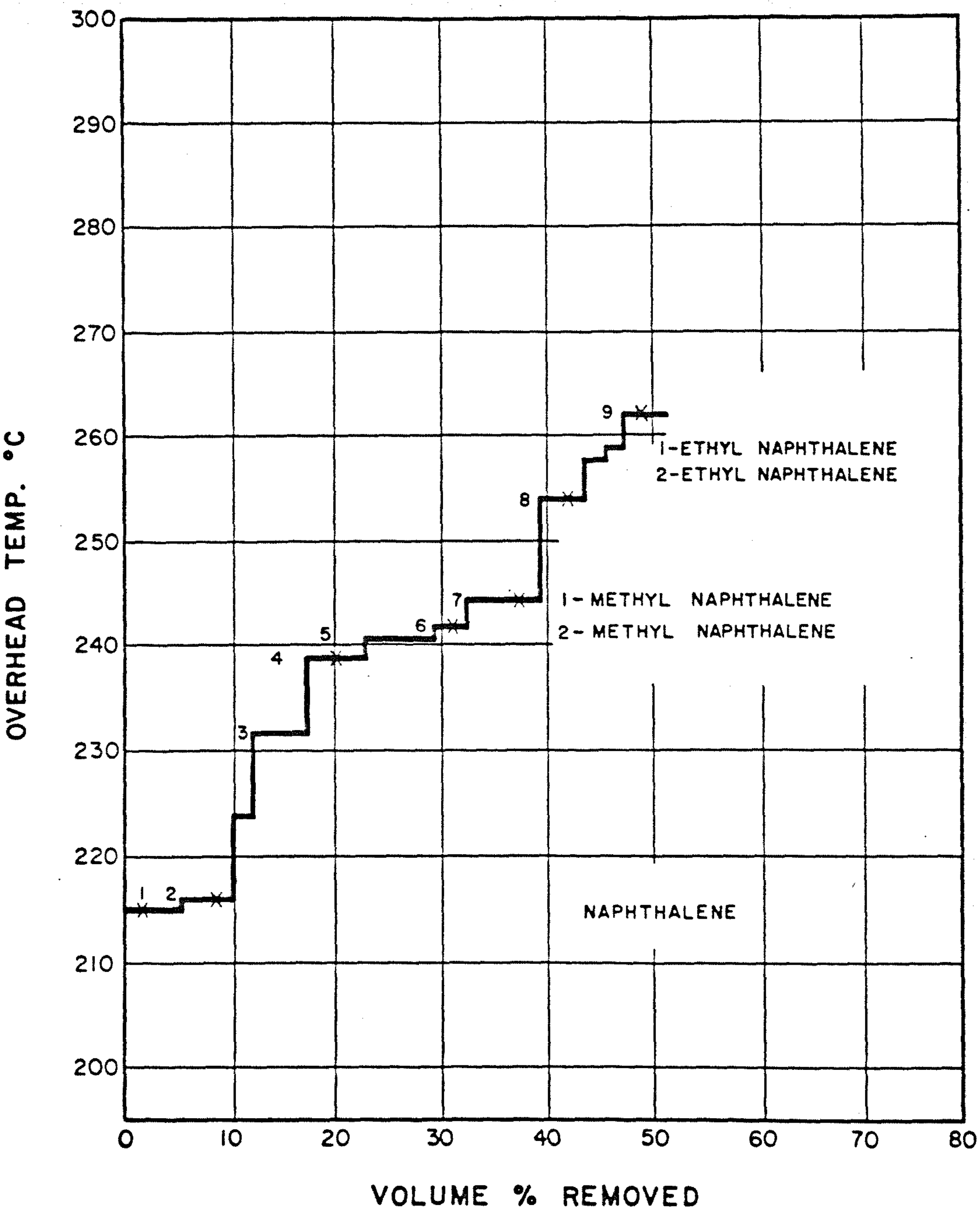


Figure 4. True Boiling Point Distillation, TBP Curve of Carbolic Oil Residue, Oldershaw-30 trays-rr 5:1.

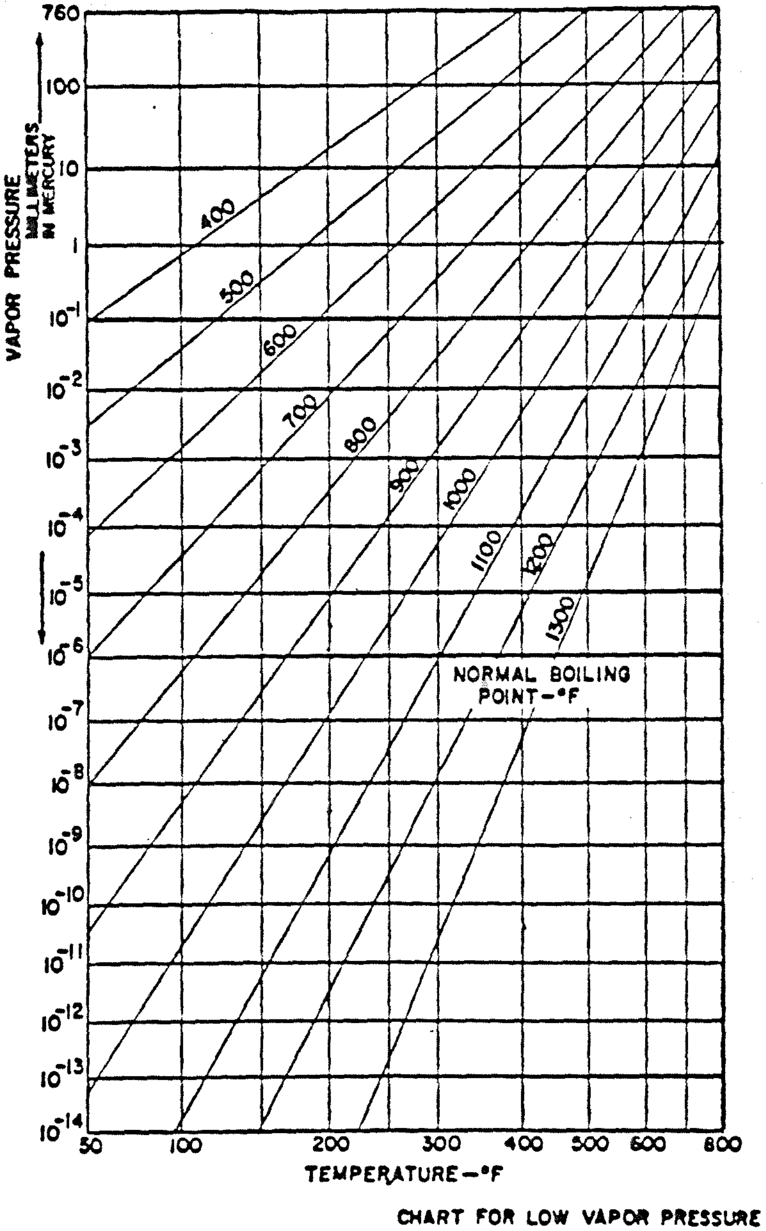


FIGURE 5. EXAMPLE MAXWELL-BONNELL CHART (16) FOR HEAVY HYDROCARBONS, K=12.

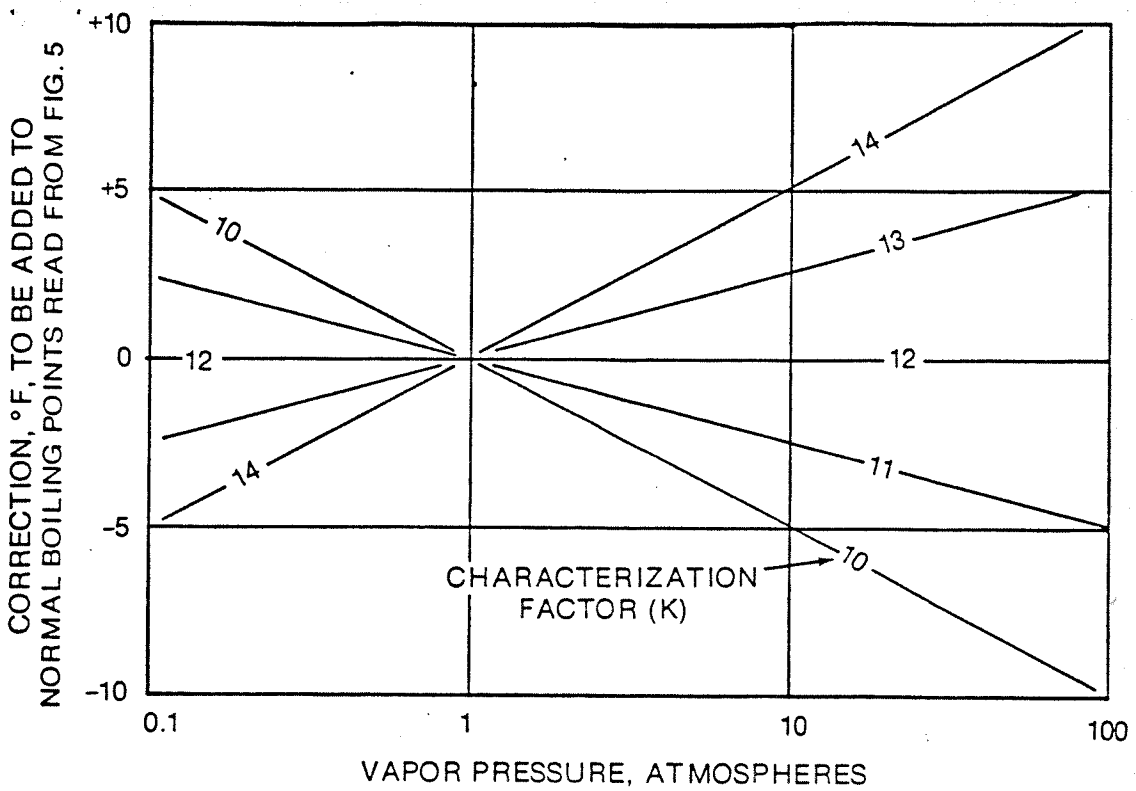


Figure 6. Boiling Point Correction for Characterization Factor, superatmosphic pressures after Maxwell and Bonnell (17).

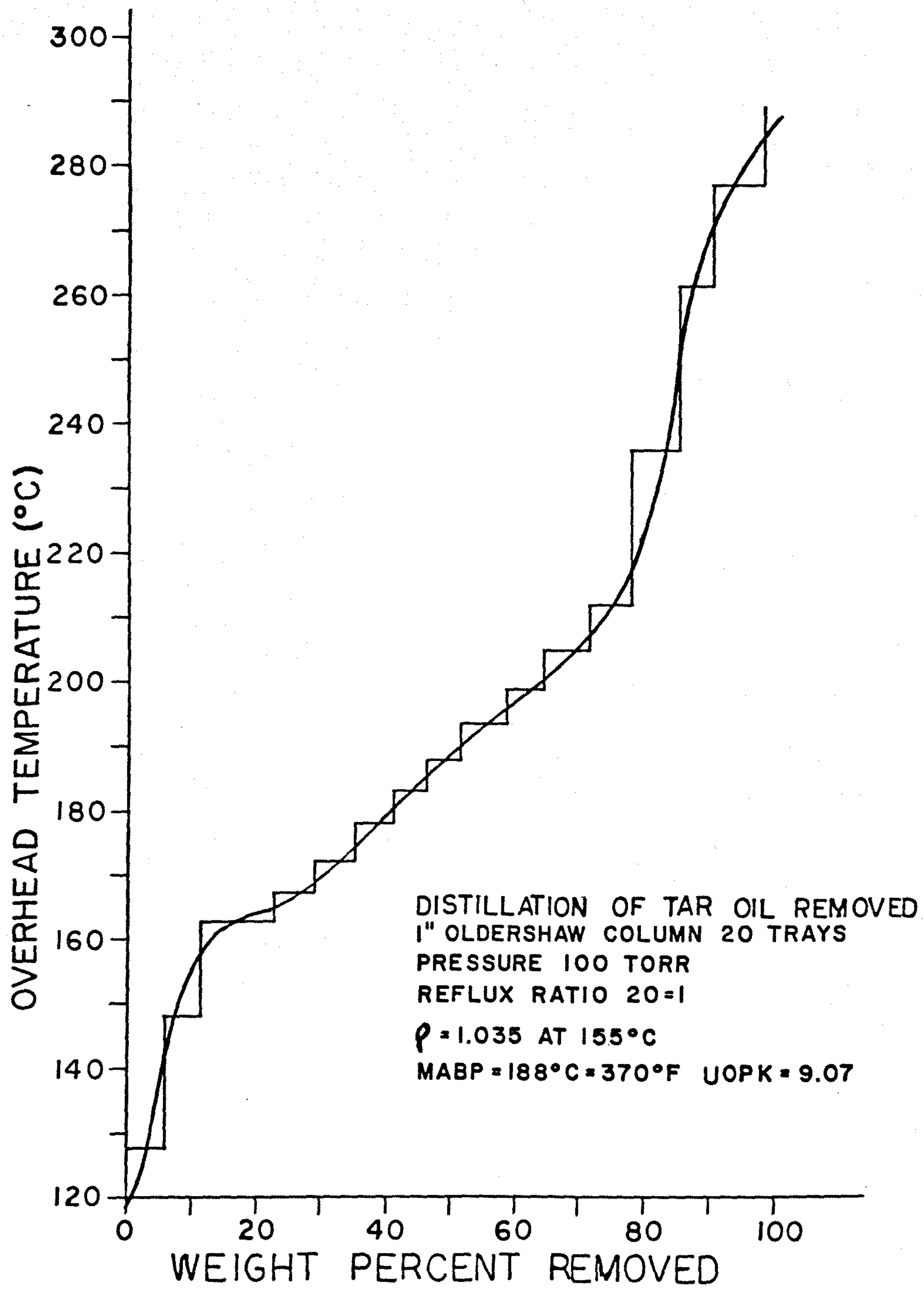


FIGURE 7

CARBOLIC OIL RESIDUE

TBP CURVE

Data From Table II

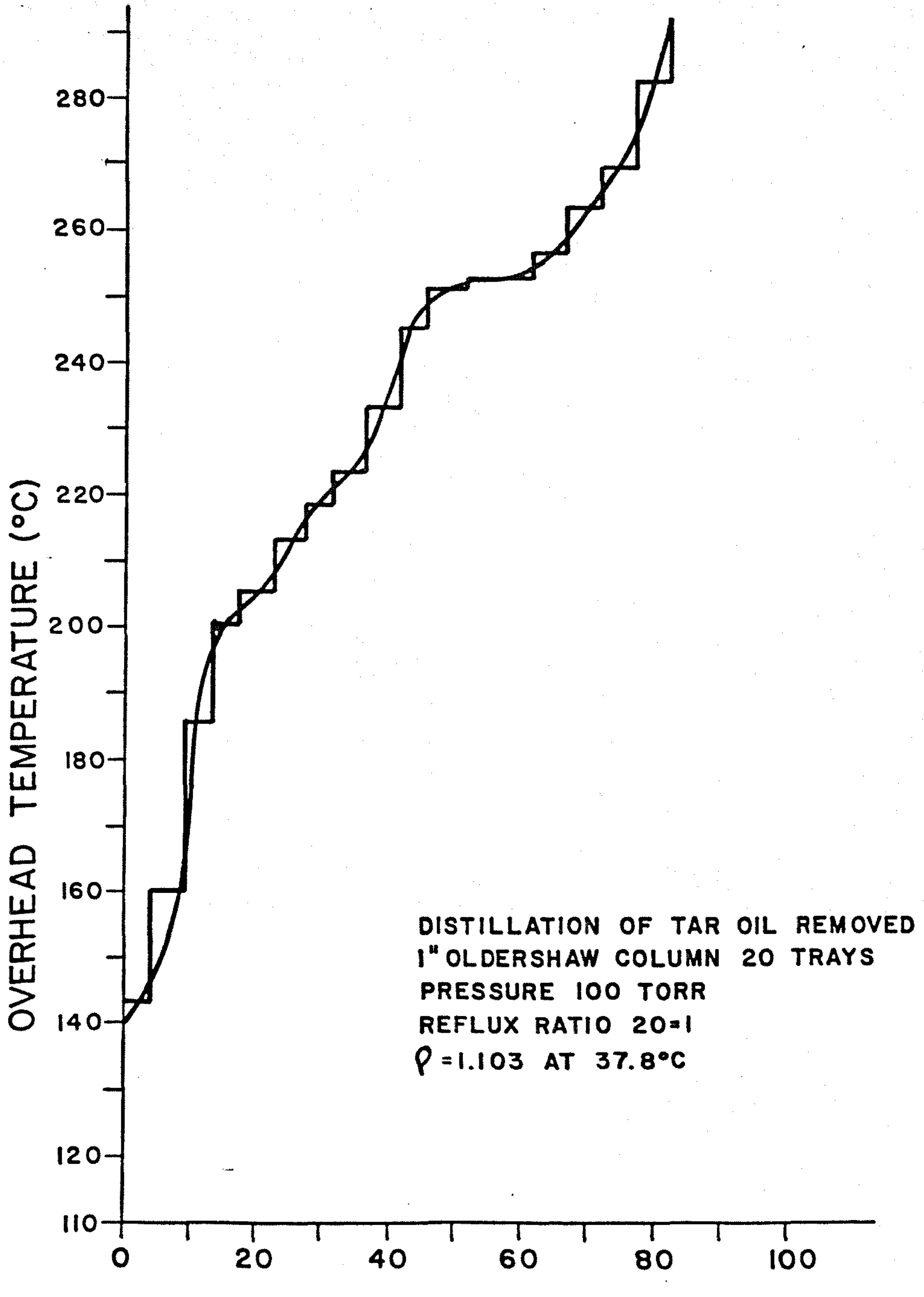


FIGURE8

LIGHT CREOSOTE OIL REFINED

TBP CURVE

Data From Table XI

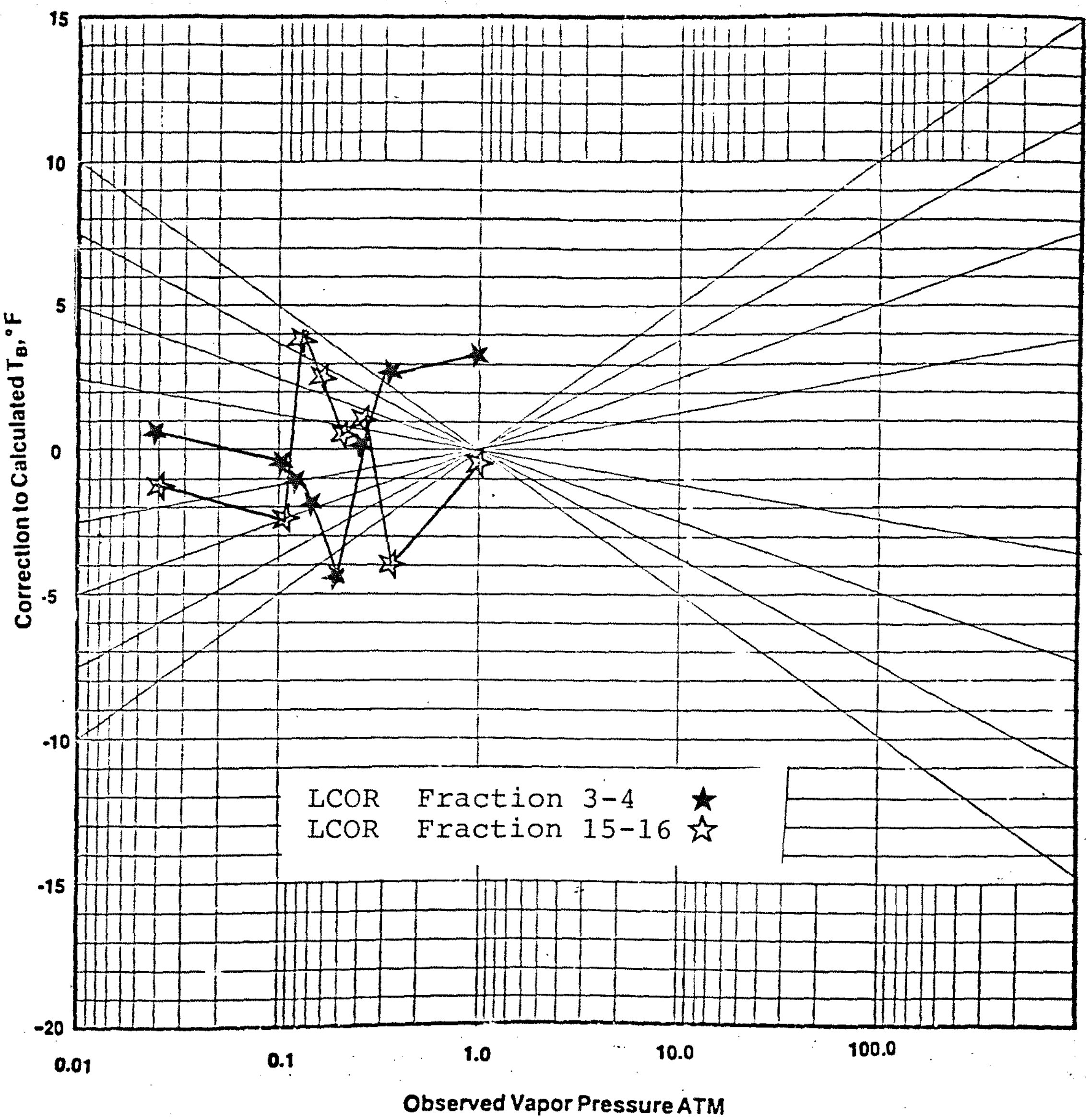


FIGURE 9. TEST OF MAXWELL-BONNELL CORRECTIONS

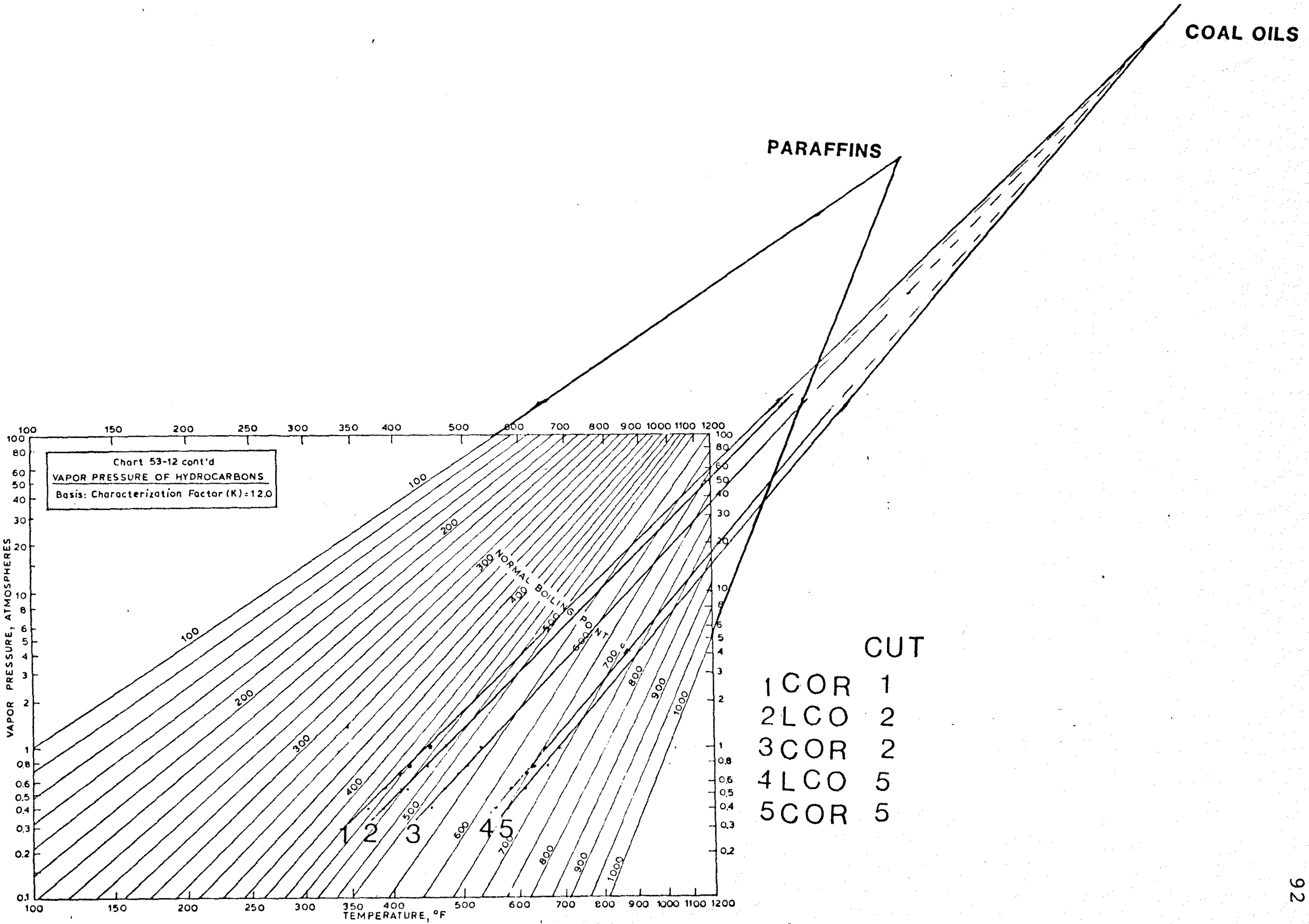


FIGURE 10 MAXWELL-BONNELL BASIC GRID FOR AROMATICS AND COAL OILS.

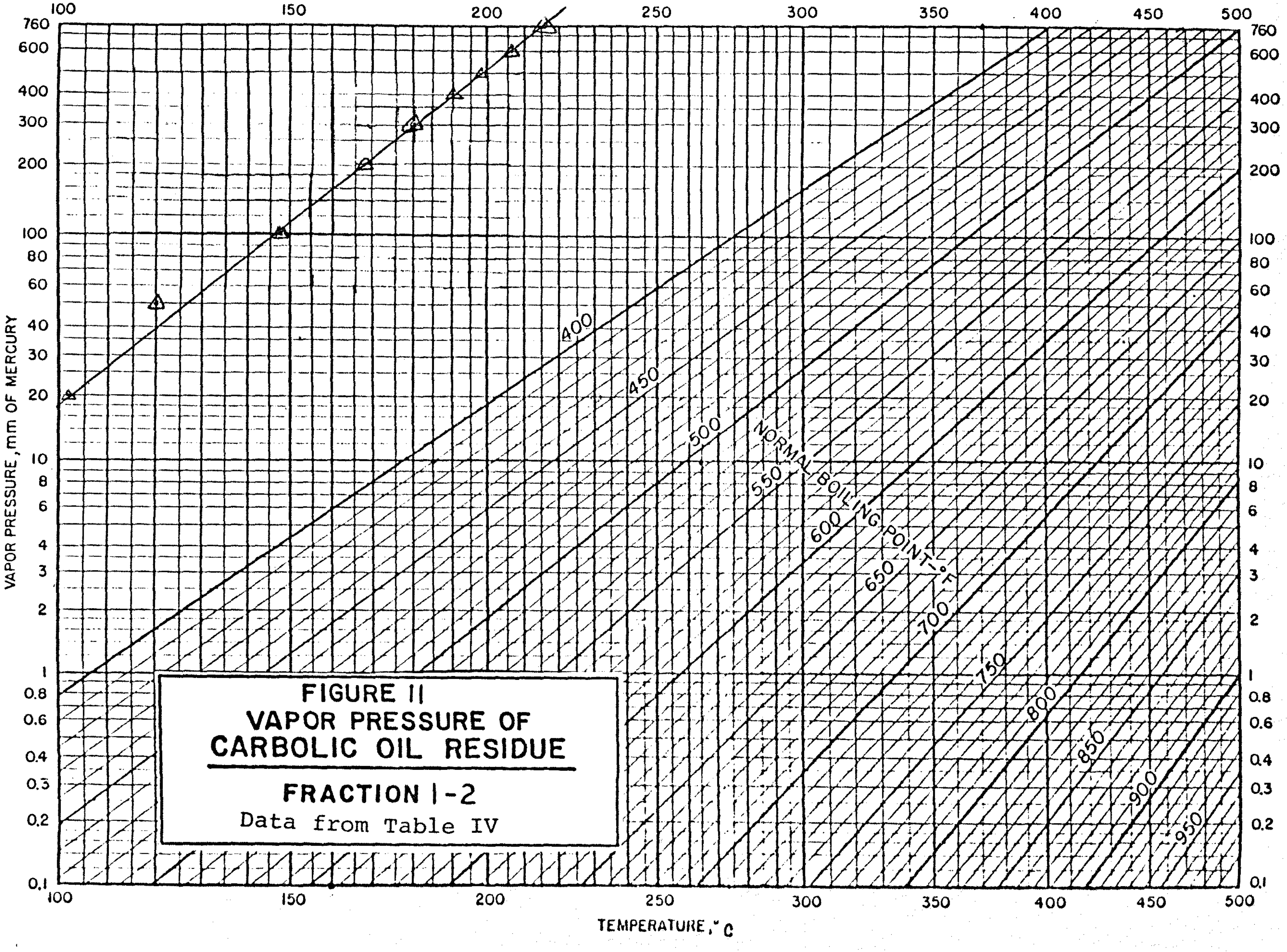


FIGURE 11
VAPOR PRESSURE OF
CARBOLIC OIL RESIDUE

FRACTION 1-2
Data from Table IV

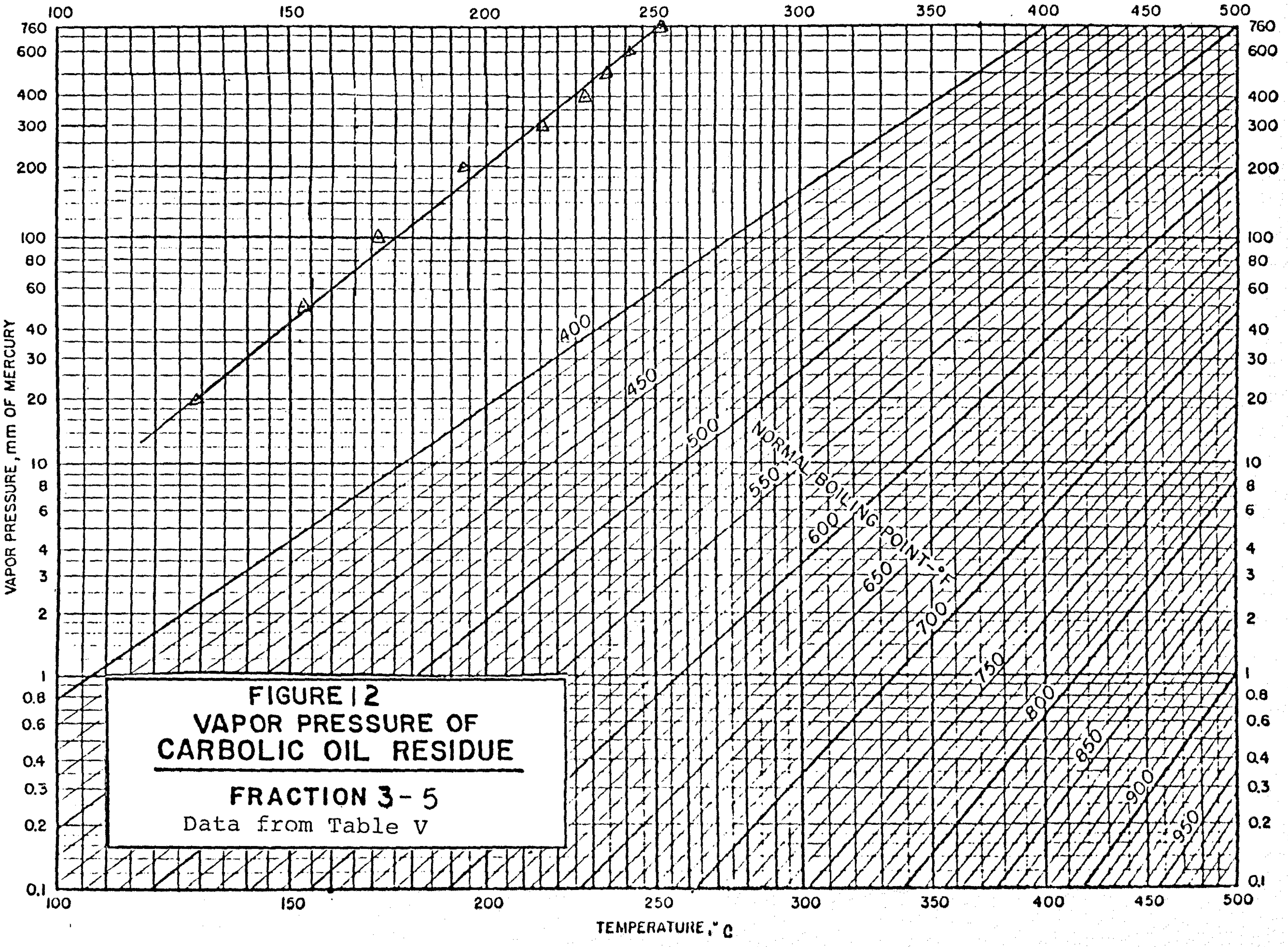


FIGURE 12
VAPOR PRESSURE OF CARBOLIC OIL RESIDUE

FRACTION 3-5
Data from Table V

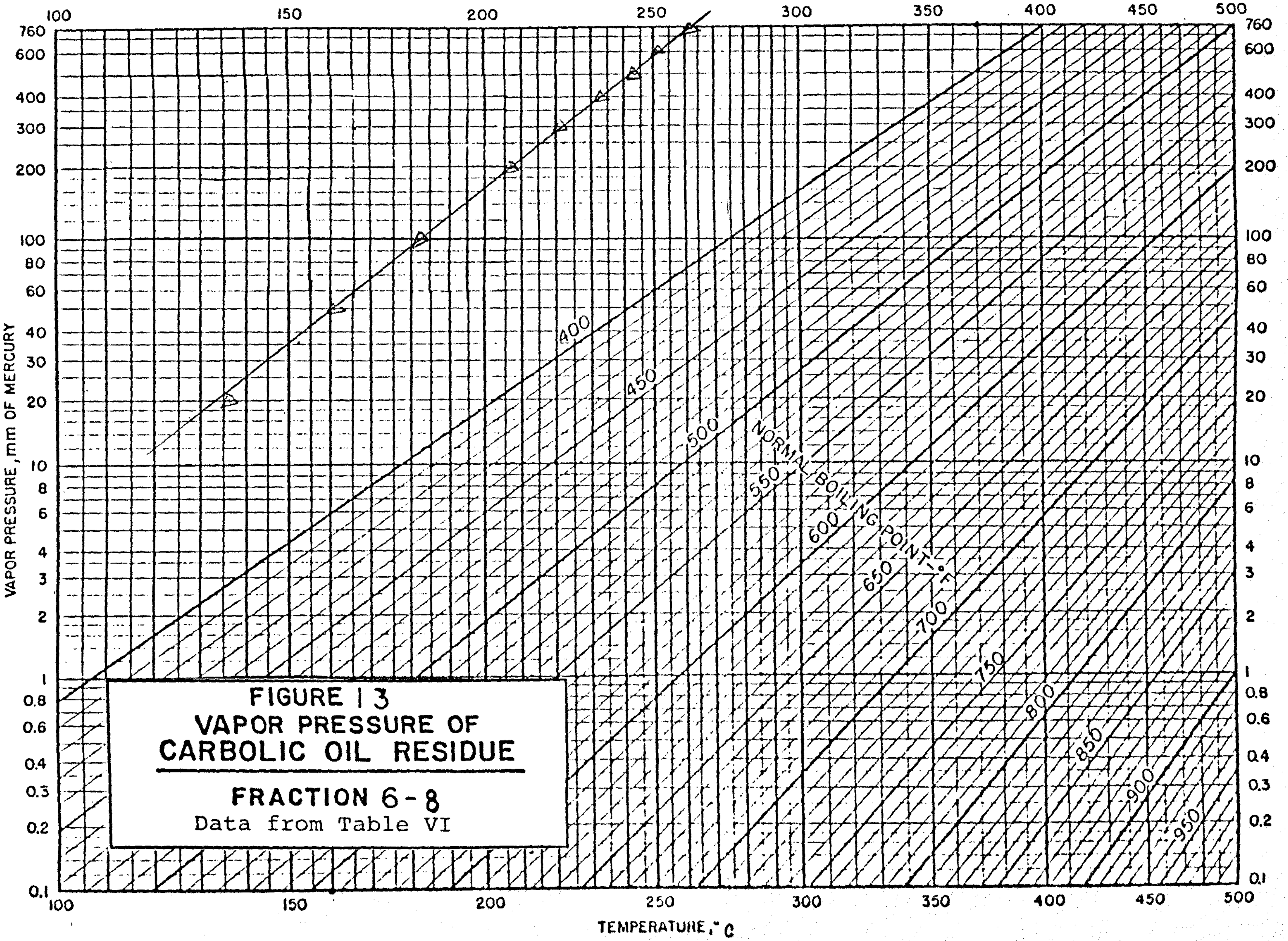


FIGURE 13
VAPOR PRESSURE OF
CARBOLIC OIL RESIDUE

FRACTION 6-8
Data from Table VI

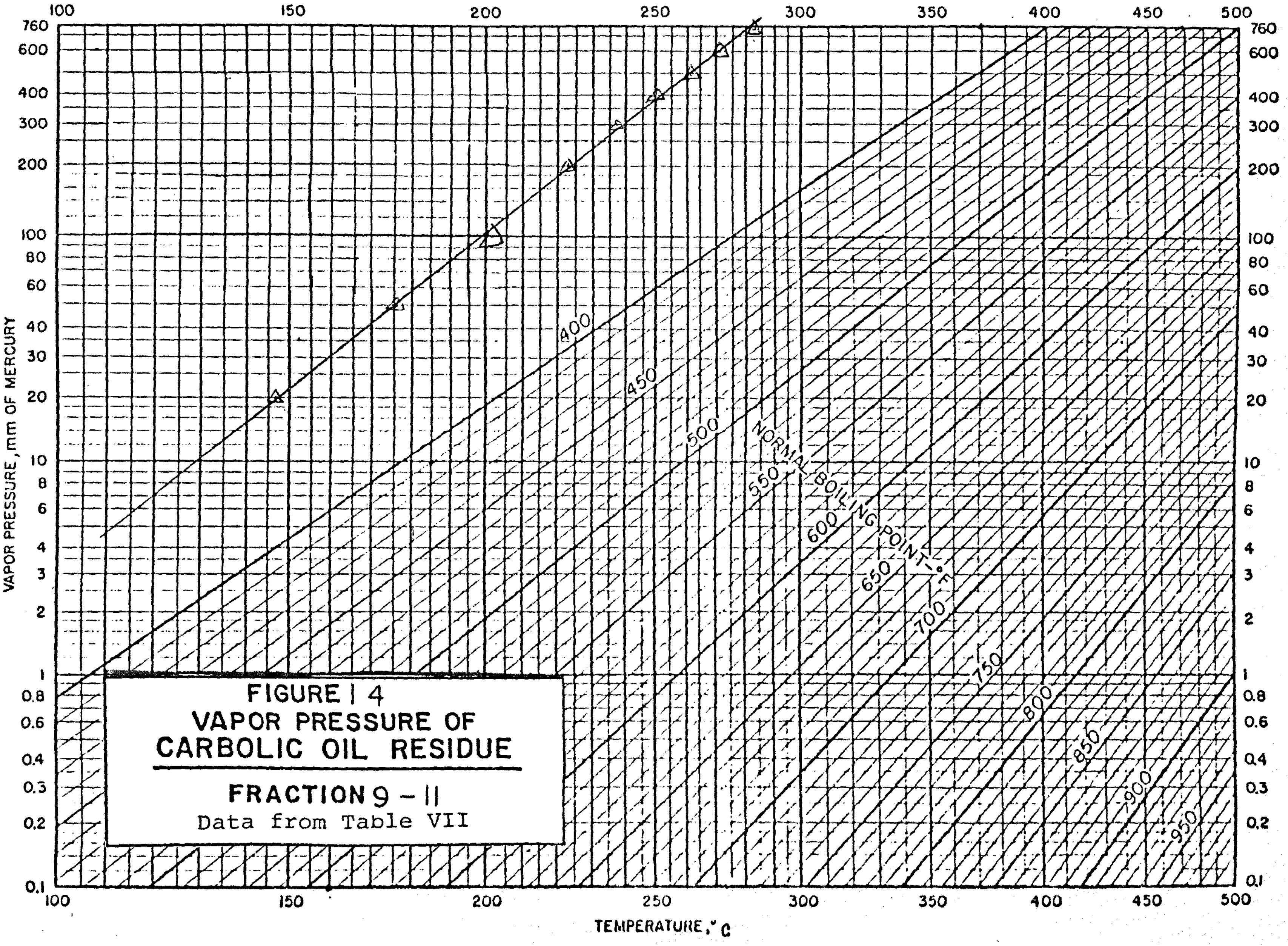


FIGURE 14
VAPOR PRESSURE OF
CARBOLIC OIL RESIDUE

FRACTION 9 – 11
Data from Table VII

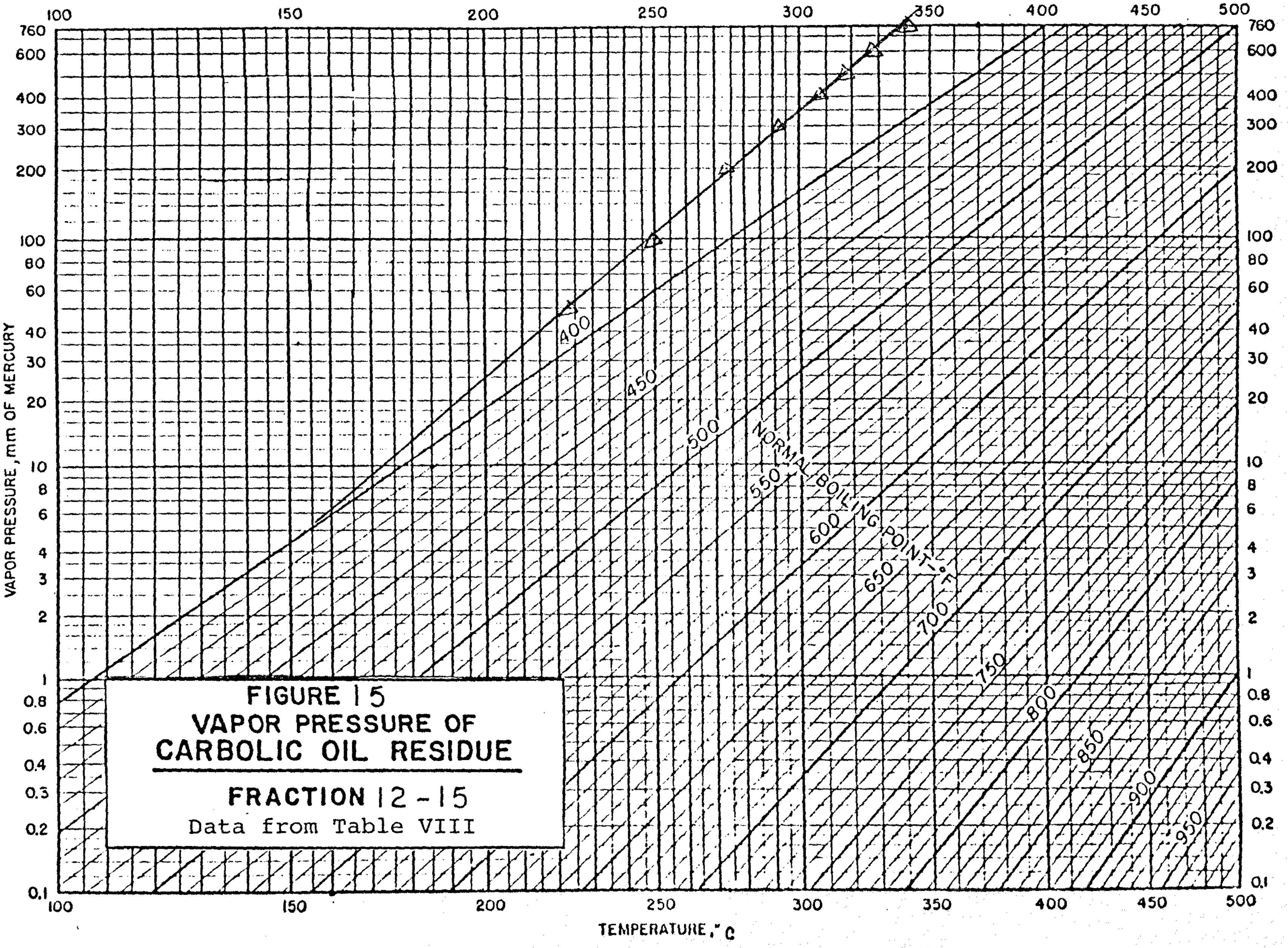


FIGURE 15
VAPOR PRESSURE OF
CARBOLIC OIL RESIDUE

FRACTION 12-15
Data from Table VIII

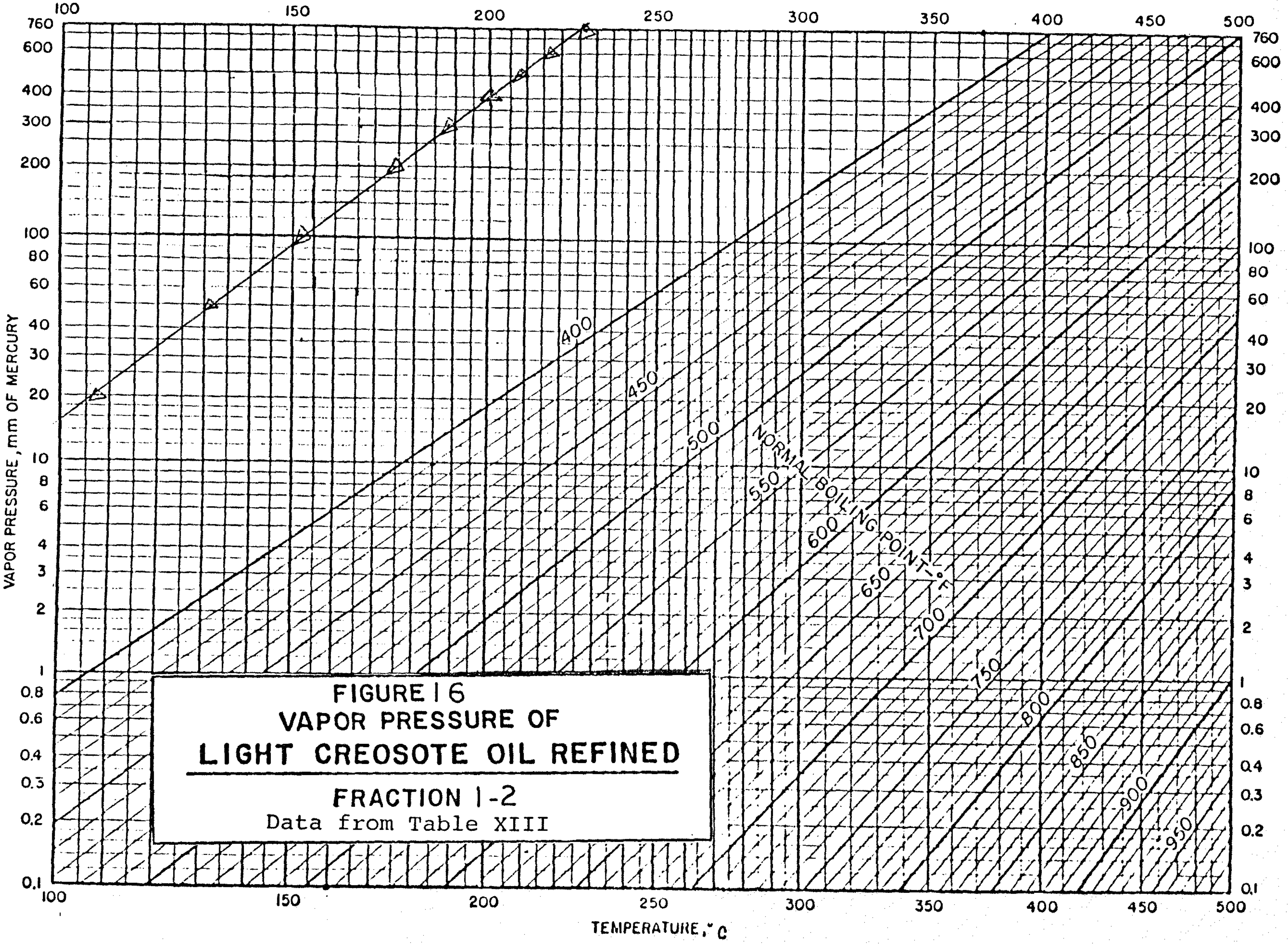


FIGURE 16

VAPOR PRESSURE OF

LIGHT CREOSOTE OIL REFINED

FRACTION 1-2

Data from Table XIII

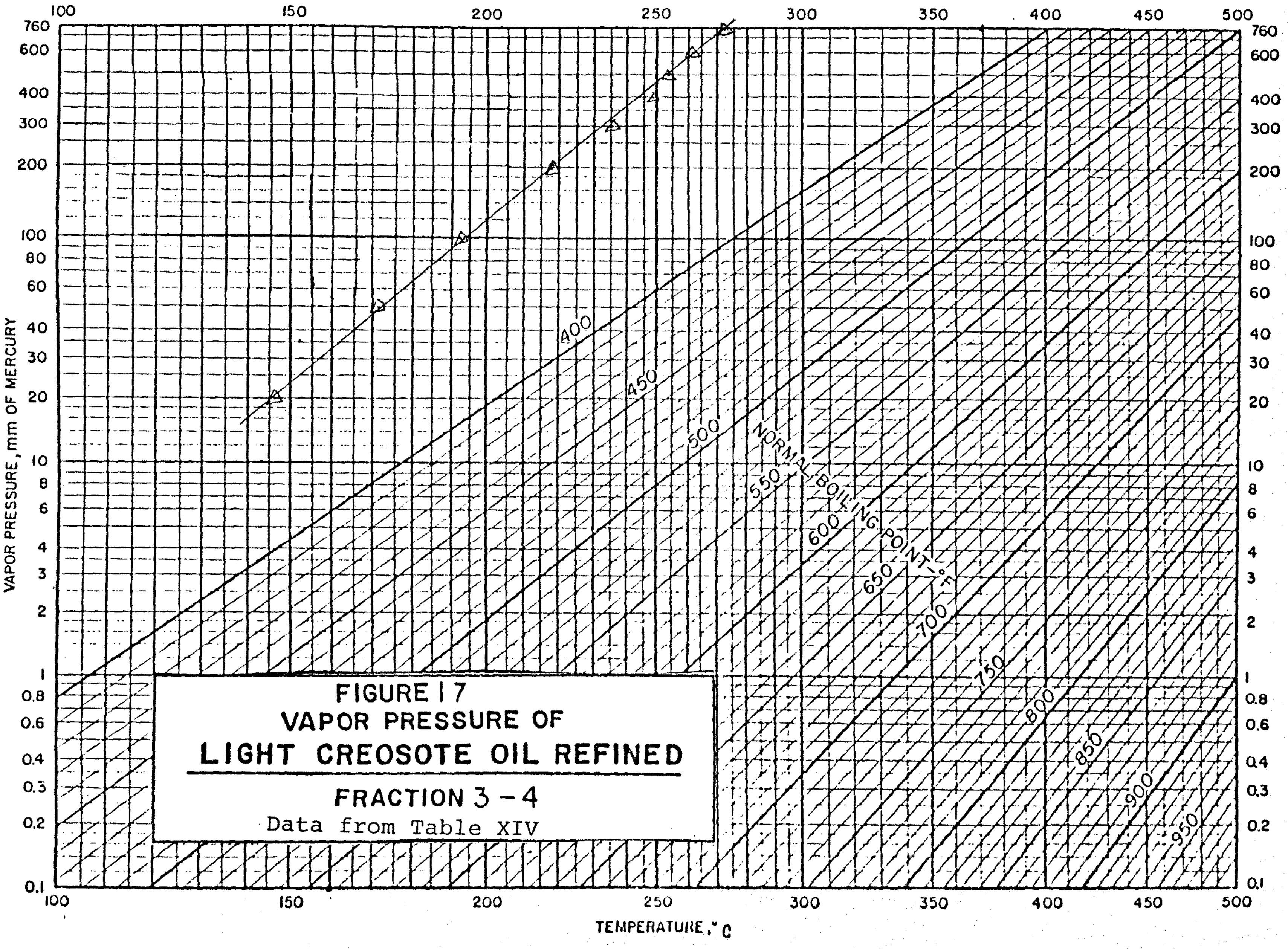


FIGURE 17
VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
FRACTION 3 - 4
Data from Table XIV

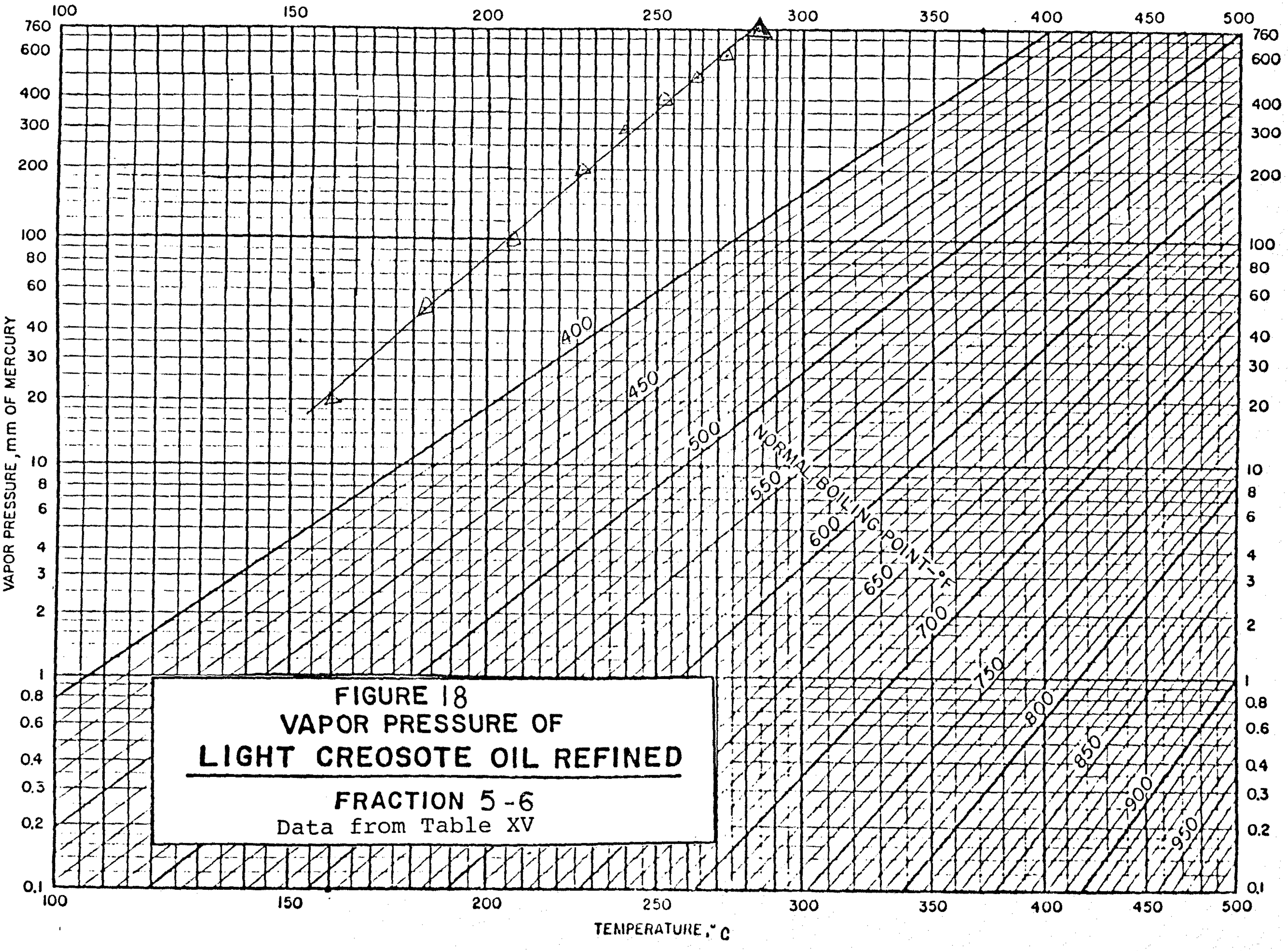


FIGURE 18
VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED

FRACTION 5-6
Data from Table XV

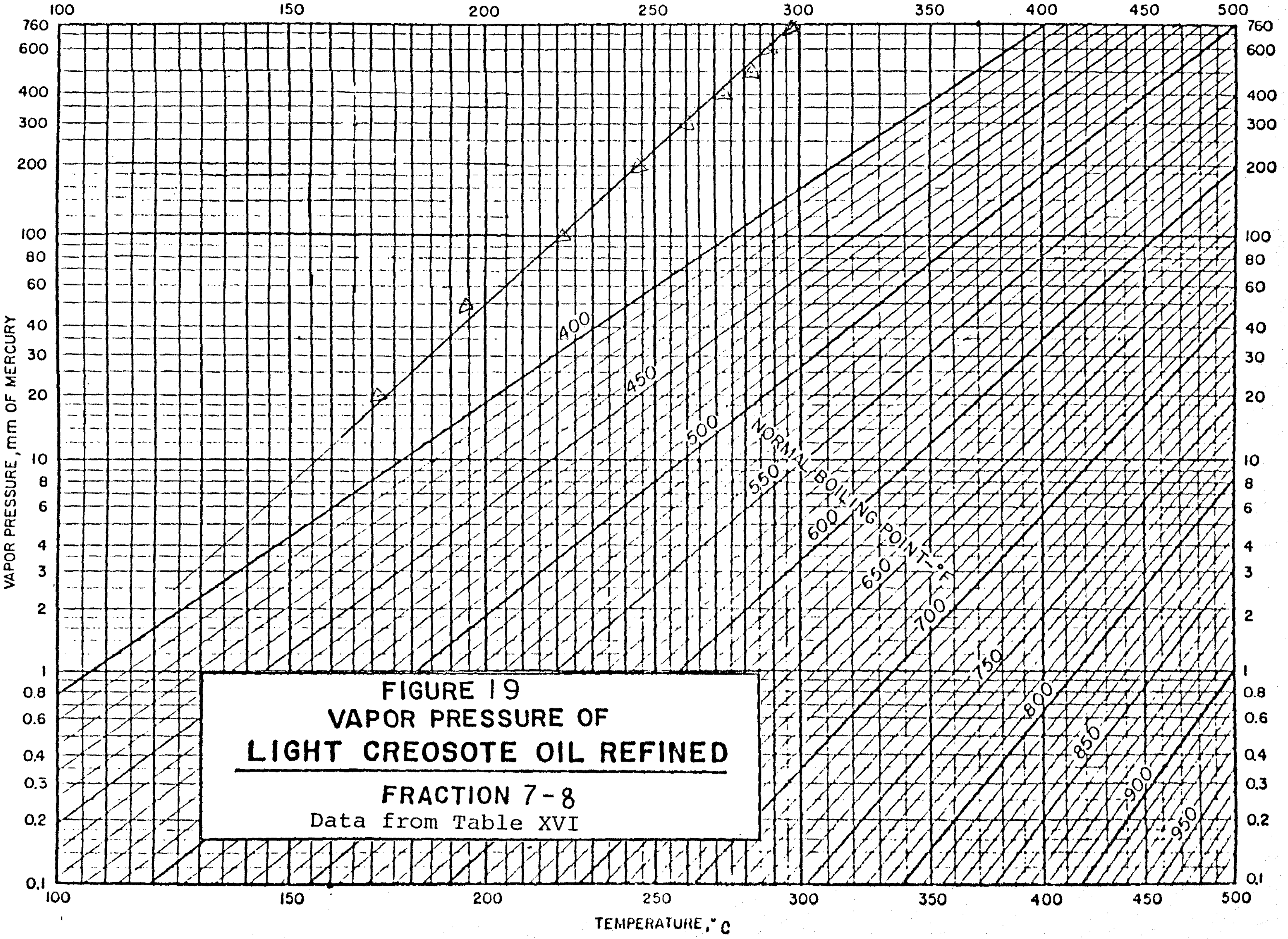


FIGURE 19
VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
FRACTION 7-8
Data from Table XVI

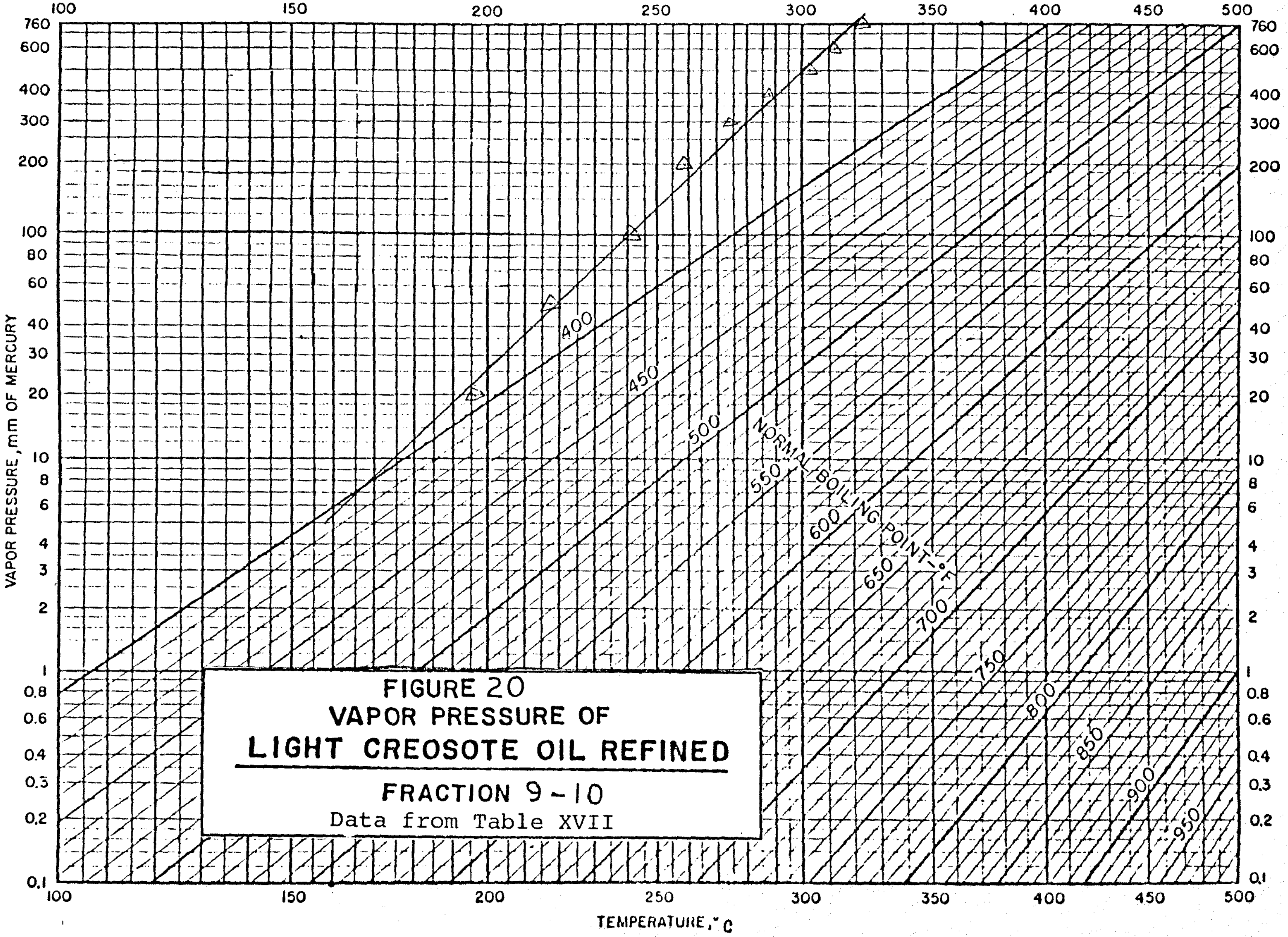


FIGURE 20
VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
FRACTION 9-10
Data from Table XVII

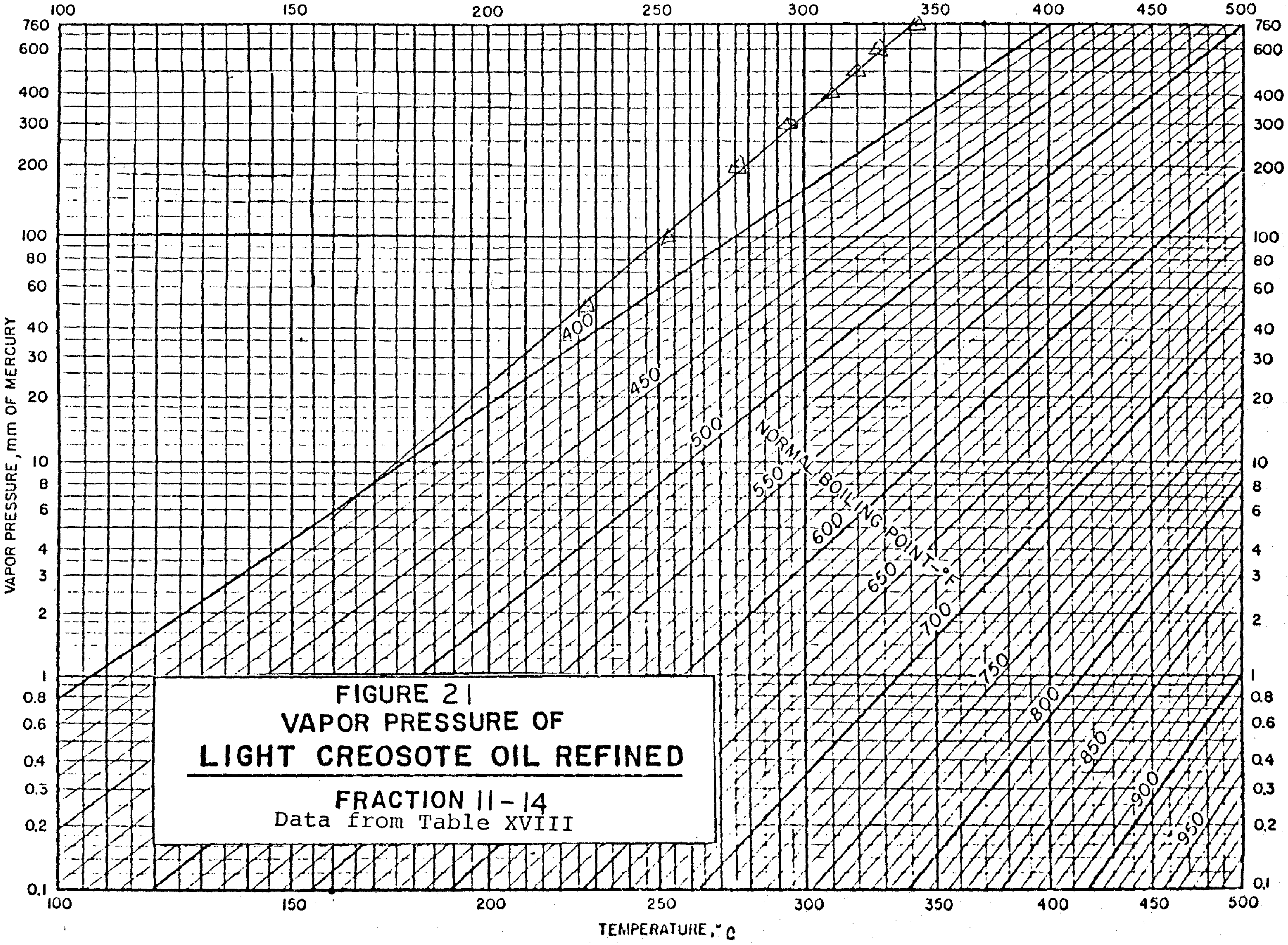


FIGURE 21
VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
FRACTION 11 - 14
Data from Table XVIII

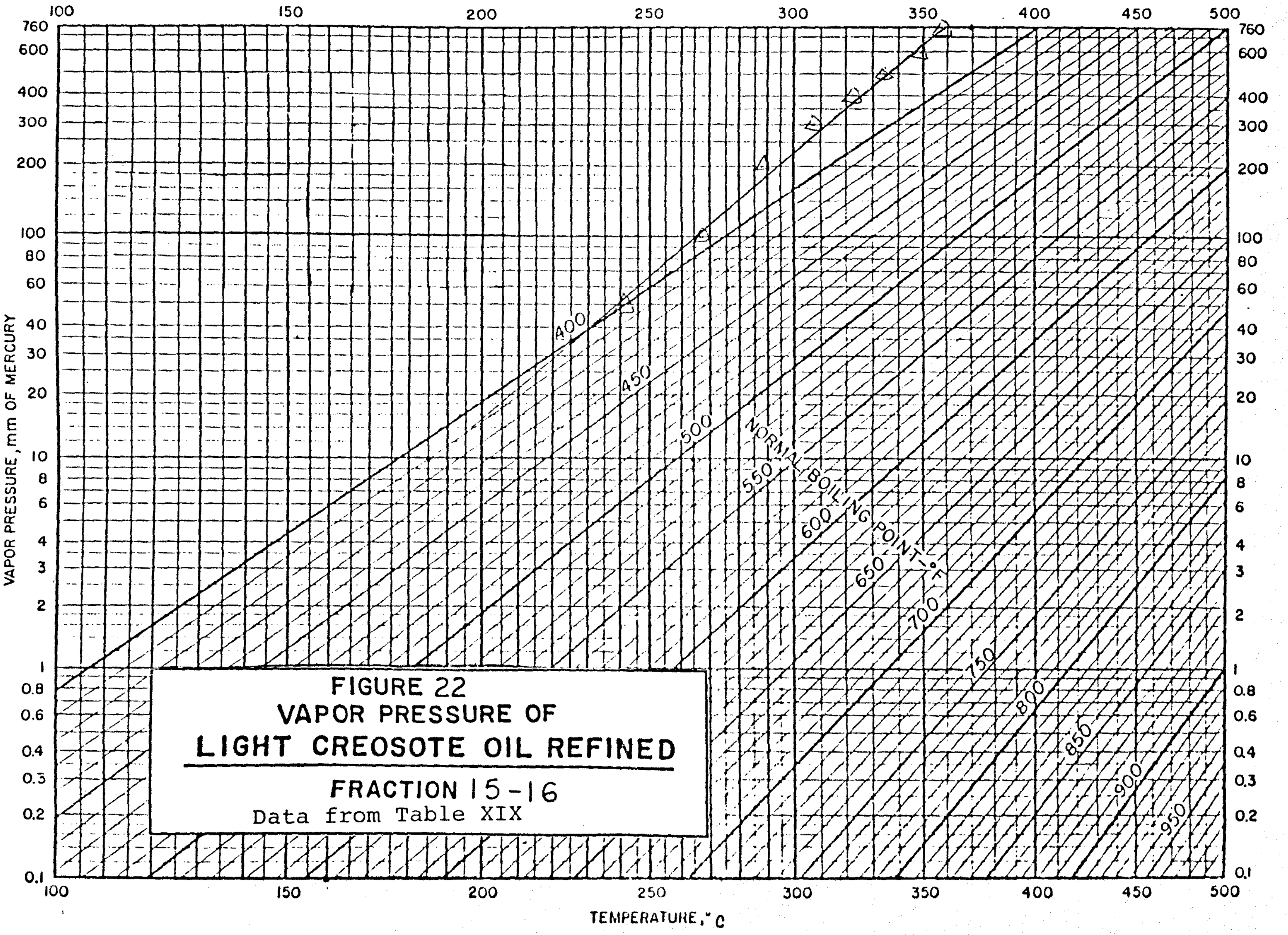


FIGURE 22
VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
FRACTION 15-16

Data from Table XIX

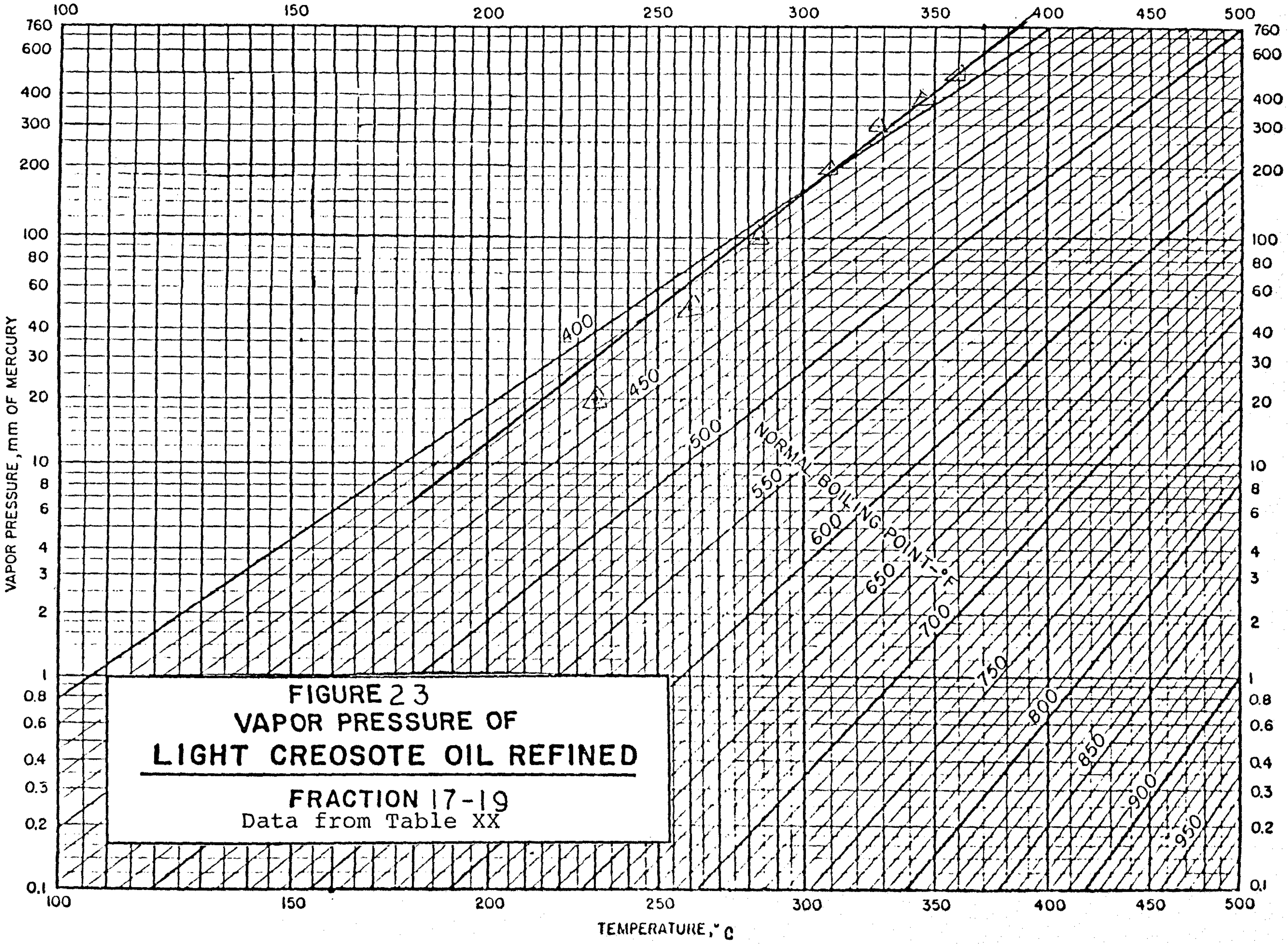


FIGURE 23
VAPOR PRESSURE OF
LIGHT CREOSOTE OIL REFINED
FRACTION 17-19
Data from Table XX

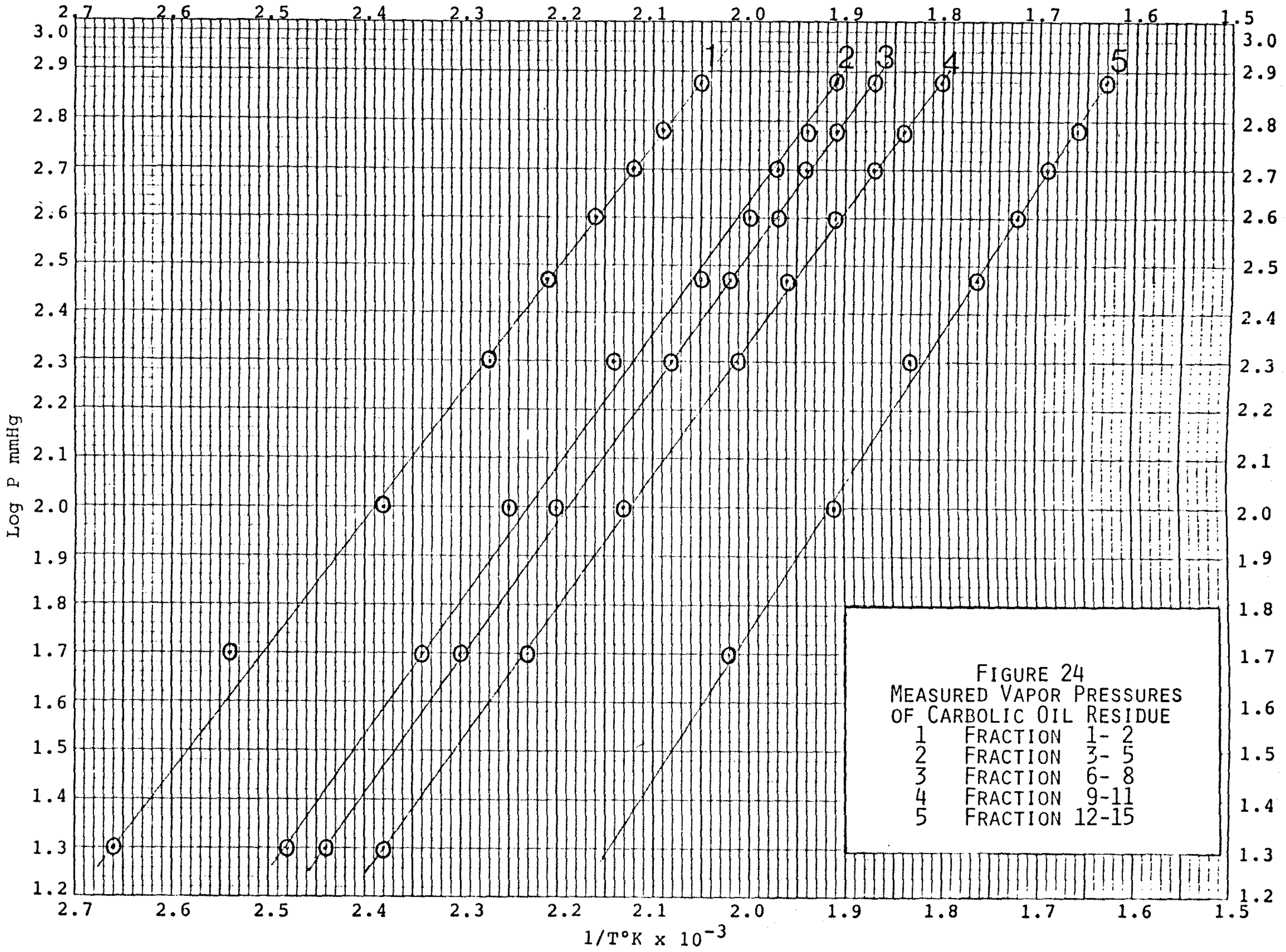


FIGURE 24
MEASURED VAPOR PRESSURES
OF CARBOLIC OIL RESIDUE
1 FRACTION 1- 2
2 FRACTION 3- 5
3 FRACTION 6- 8
4 FRACTION 9-11
5 FRACTION 12-15

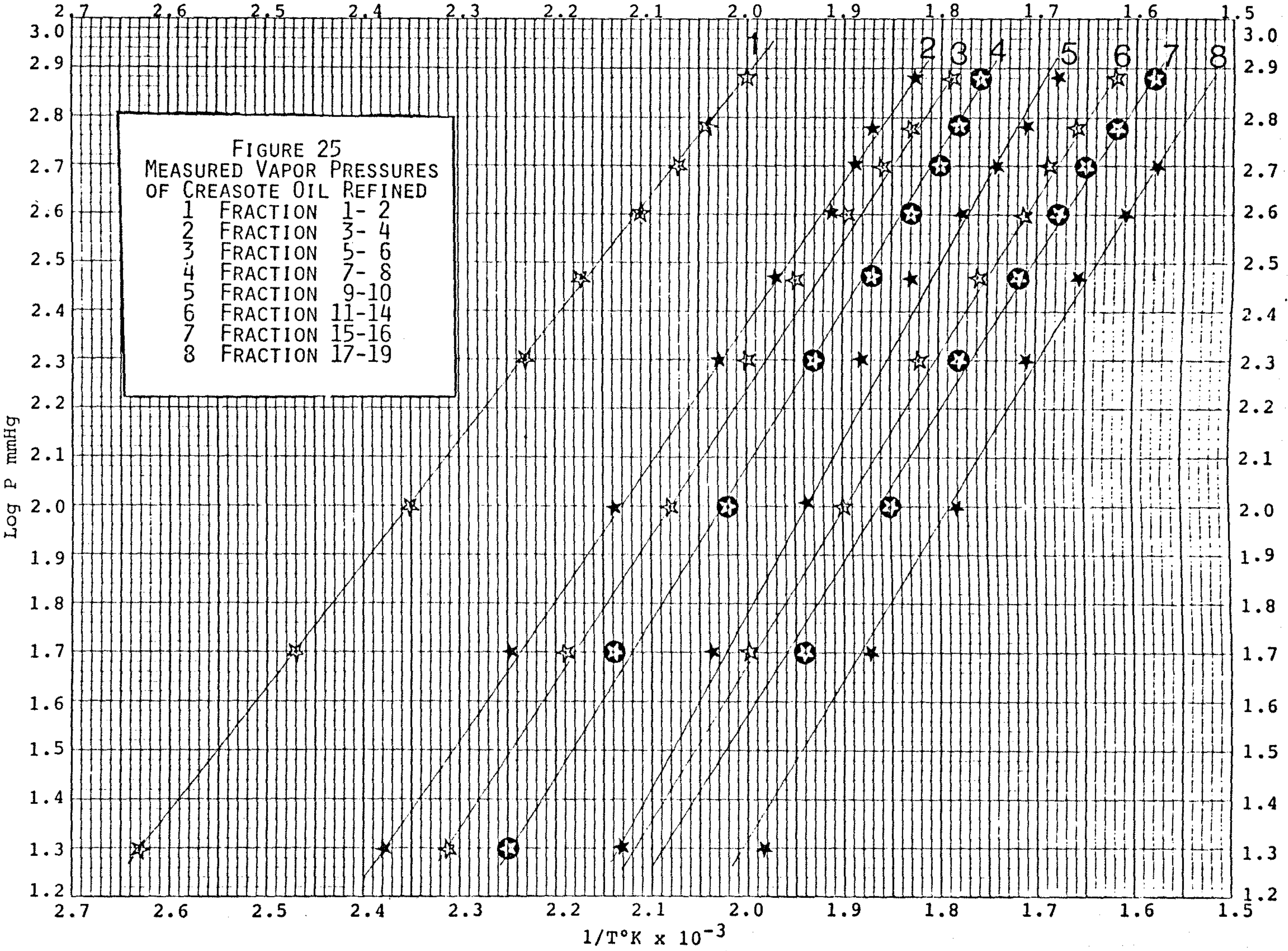
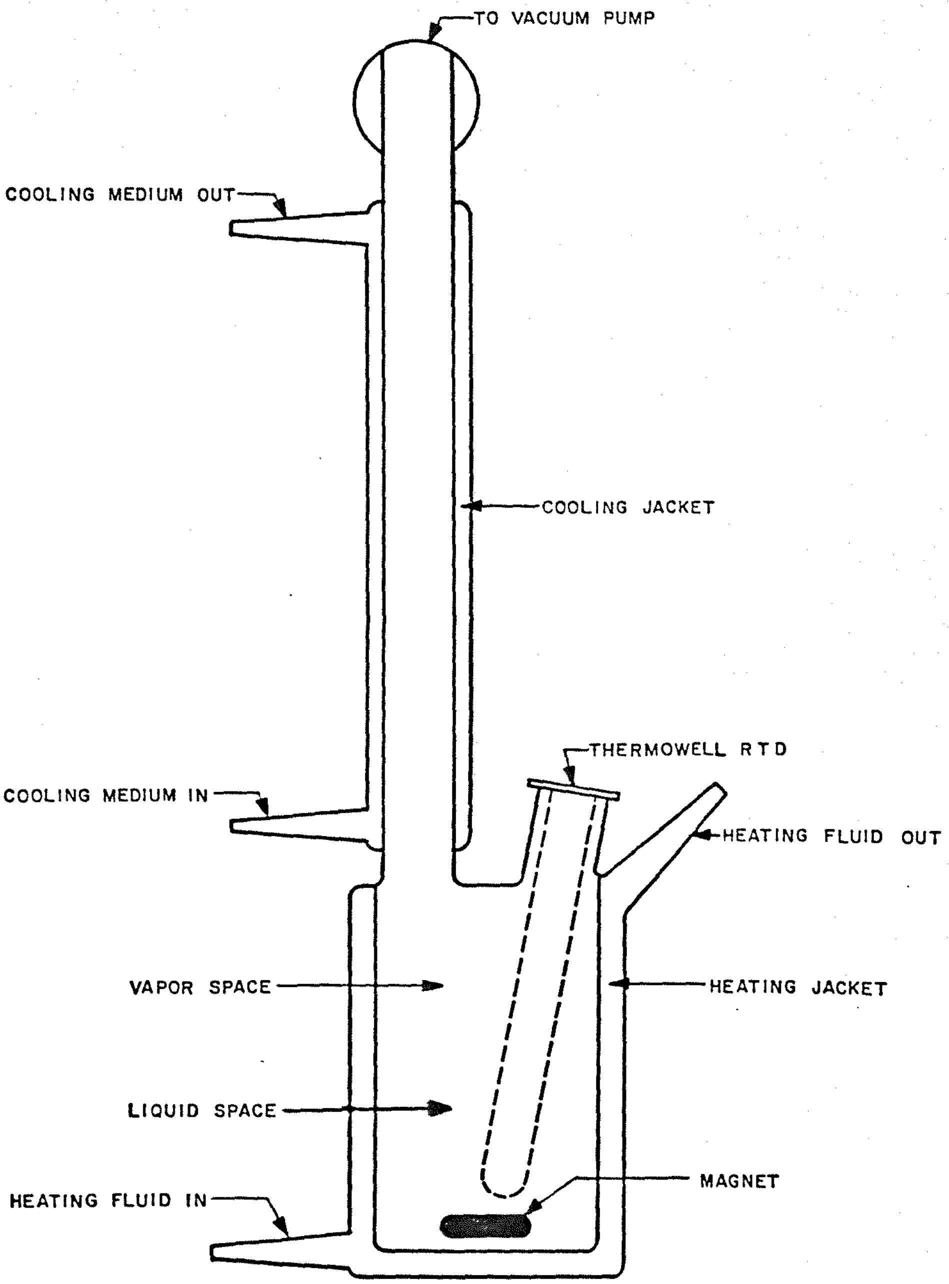


FIGURE 25
MEASURED VAPOR PRESSURES
OF CREASOTE OIL REFINED

FIGURE 26



VAPOR PRESSURE STILL

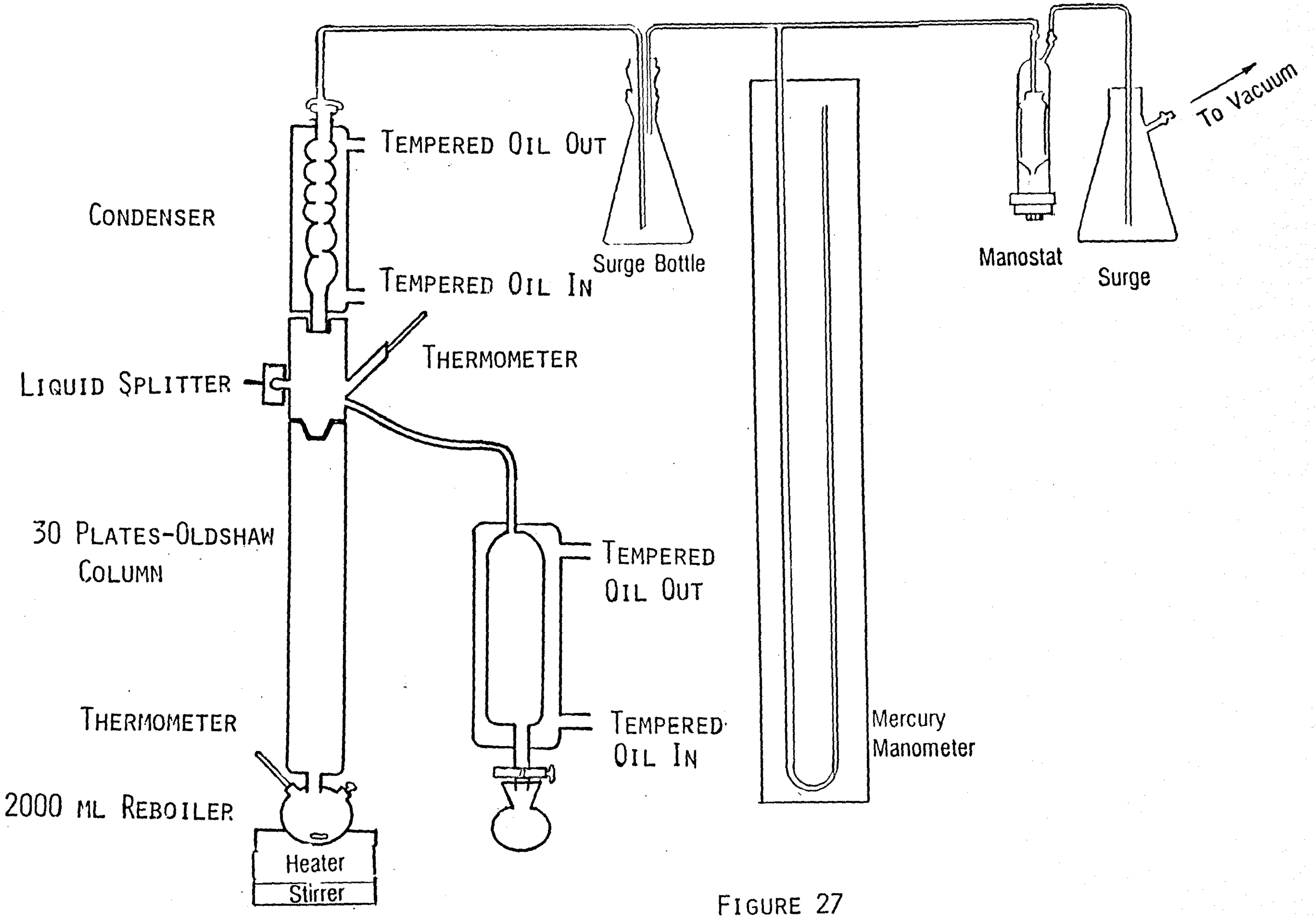


FIGURE 27

EQUIPMENT SET UP FOR THE DISTILLATIONS

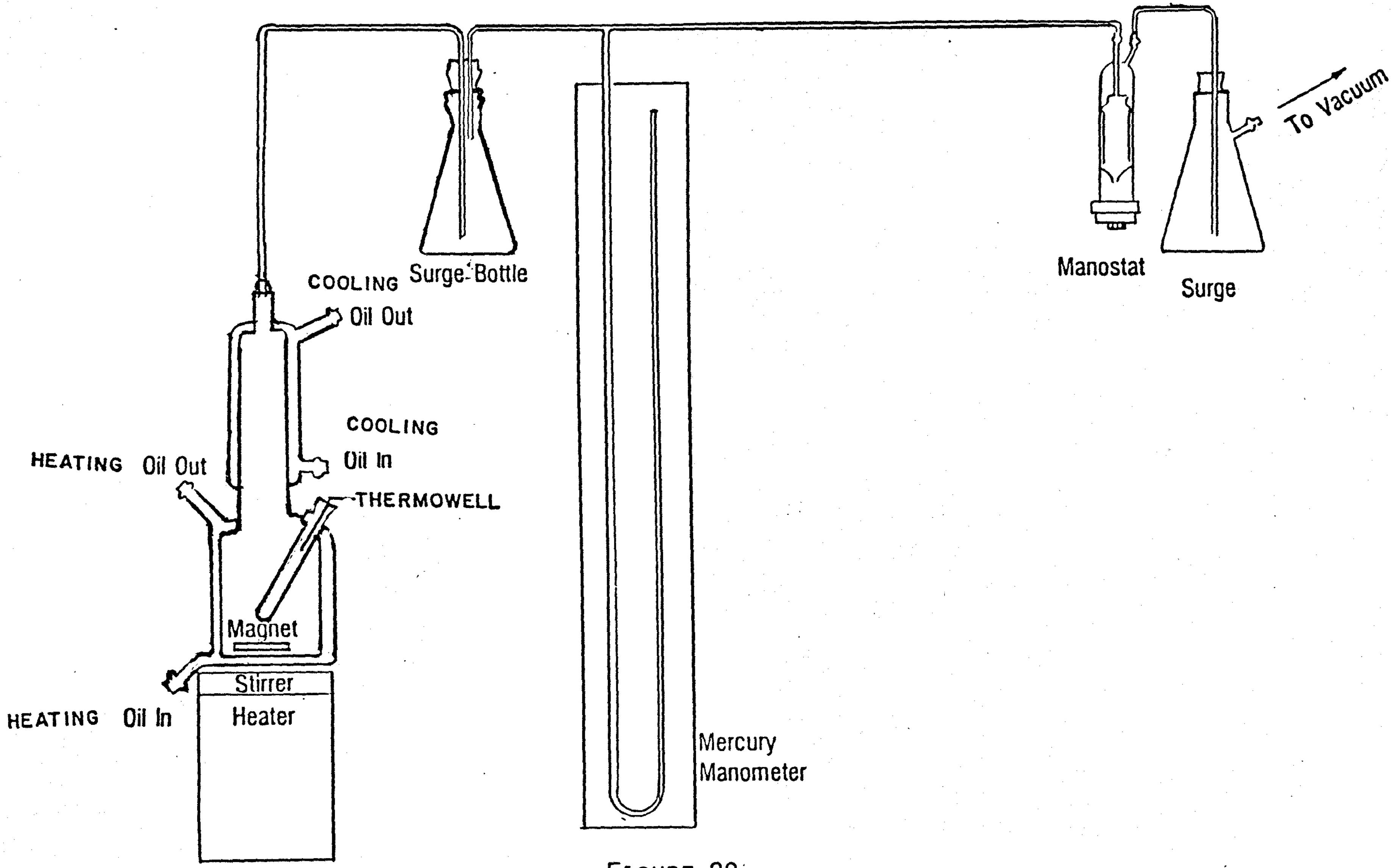


FIGURE 28

EQUIPMENT SET UP FOR
VAPOR PRESSURE MEASUREMENTS

APPENDIX 3

Table A
Computer Results
Carbolic Oil Residue
Fraction 1-2

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
879.56995	0.99842	615.65765	0.1624E-02	0.1137E-02	613.81128
861.56995	0.78947	602.33563	0.1660E-02	0.1161E-02	600.63312
849.14996	0.65789	592.45319	0.1688E-02	0.1178E-02	591.55597
834.02997	0.52632	580.87054	0.1722E-02	0.1199E-02	580.52283
815.31000	0.39474	566.71185	0.1765E-02	0.1227E-02	566.88898
793.52997	0.26316	548.10413	0.1824E-02	0.1260E-02	551.06305
757.52997	0.13158	519.48401	0.1925E-02	0.1320E-02	524.99005
708.56995	0.06579	494.20117	0.2023E-02	0.1411E-02	489.70096
675.63000	0.02632	465.79880	0.2147E-02	0.1480E-02	466.06842

SLOPE	INTERCEPT
1.50487	-0.0000818

Table B
Computer Results
Carbolic Oil Residue
Fraction 3-4-5

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
944.54999	0.99237	615.30383	0.1625E-02	0.1059E-02	613.81287
926.37000	0.78947	602.33563	0.1660E-02	0.1079E-02	601.52295
913.58997	0.65789	592.45319	0.1688E-02	0.1095E-02	592.89514
900.63000	0.52632	580.87054	0.1722E-02	0.1110E-02	584.15558
879.56995	0.39474	566.71185	0.1765E-02	0.1137E-02	569.97467
840.51001	0.26316	548.10413	0.1824E-02	0.1190E-02	543.74200
800.72998	0.13158	519.48401	0.1925E-02	0.1249E-02	517.11676
768.51001	0.06579	494.20117	0.2023E-02	0.1301E-02	495.61853
724.58997	0.02632	465.79880	0.2147E-02	0.1380E-02	466.40985

SLOPE	INTERCEPT
1.60205	-0.0000669

Table C
Computer Results
Carbolic Oil Residue
Fraction 6-7-8

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
964.17004	0.99421	615.41168	0.1625E-02	0.1037E-02	615.22235
943.64996	0.78947	602.33563	0.1660E-02	0.1060E-02	601.53900
929.78998	0.65789	592.45319	0.1688E-02	0.1076E-02	592.31189
912.51001	0.52632	580.87054	0.1722E-02	0.1096E-02	580.82513
890.54999	0.39474	566.71185	0.1765E-02	0.1123E-02	566.25452
865.52997	0.26316	548.10413	0.1824E-02	0.1155E-02	549.69073
819.63000	0.13158	519.48401	0.1925E-02	0.1220E-02	519.40619
782.54999	0.06579	494.20117	0.2023E-02	0.1278E-02	495.03717
736.64996	0.02632	465.79880	0.2147E-02	0.1357E-02	464.98996

SLOPE	INTERCEPT
1.63939	-0.0000749

Table D
Computer Results
Carbolic Oil Residue
Fraction 9-10-11

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1000.17004	0.99474	615.44250	0.1625E-02	0.9998E-03	615.69904
980.18994	0.78947	602.33563	0.1660E-02	0.1020E-02	603.25116
961.64996	0.65789	592.45319	0.1688E-02	0.1040E-02	591.70599
942.57001	0.52632	580.87054	0.1722E-02	0.1061E-02	579.83008
919.52997	0.39474	566.71185	0.1765E-02	0.1088E-02	565.49664
893.60999	0.26316	548.10413	0.1824E-02	0.1119E-02	549.38129
845.54999	0.13158	519.48401	0.1925E-02	0.1183E-02	519.52789
806.84998	0.06579	494.20117	0.2023E-02	0.1239E-02	495.51419
757.52997	0.02632	465.79880	0.2147E-02	0.1320E-02	464.94376

SLOPE	INTERCEPT
1.64443	-0.0000200

Table E
Computer Results
Carbolic Oil Residue
Fraction 12-15

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1104.75000	0.99618	615.52710	0.1625E-02	0.9052E-03	615.19391
1082.60999	0.78947	602.33563	0.1660E-02	0.9237E-03	602.42395
1065.51001	0.65789	592.45319	0.1688E-02	0.9385E-03	592.57379
1046.96997	0.52632	580.87054	0.1722E-02	0.9551E-03	581.90662
1020.33002	0.39474	566.71185	0.1765E-02	0.9801E-03	566.60199
984.87000	0.26316	548.10413	0.1824E-02	0.1015E-02	546.27185
940.22992	0.13158	519.48401	0.1925E-02	0.1064E-02	520.74603
893.25000	0.06579	494.20117	0.2023E-02	0.1120E-02	493.96304

SLOPE	INTERCEPT
1.86137	-0.0000594

Table F
Computer Results
Light Creosote Oil Refined
Fraction 1-2

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
899.54999	0.99789	615.62695	0.1624E-02	0.1112E-02	614.39722
883.34998	0.78947	602.33563	0.1660E-02	0.1132E-02	603.00348
867.51001	0.65789	592.45319	0.1688E-02	0.1153E-02	591.87500
852.56995	0.52632	580.87054	0.1722E-02	0.1173E-02	581.38959
830.60999	0.39474	566.71185	0.1765E-02	0.1204E-02	565.99652
805.58997	0.26316	548.10413	0.1824E-02	0.1241E-02	548.48615
765.81000	0.13158	519.48401	0.1925E-02	0.1306E-02	520.70642
728.54999	0.06579	494.20117	0.2023E-02	0.1373E-02	494.75360
685.52997	0.02632	465.79880	0.2147E-02	0.1459E-02	464.86917

SLOPE	INTERCEPT
1.50848	-0.0000493

Table G
Computer Results
Light Creosote Oil Residue
Fraction 3-4

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
981.63007	0.99776	615.61926	0.1624E-02	0.1019E-02	612.39160
962.01001	0.78947	602.33563	0.1660E-02	0.1039E-02	599.45551
950.48993	0.65789	592.45319	0.1688E-02	0.1052E-02	591.87396
940.58997	0.52632	580.87054	0.1722E-02	0.1063E-02	585.36694
915.02997	0.39474	566.71185	0.1765E-02	0.1093E-02	568.60187
885.33002	0.26316	548.10413	0.1824E-02	0.1130E-02	549.18475
839.78998	0.13158	519.48401	0.1925E-02	0.1191E-02	519.54321
799.64996	0.06579	494.20117	0.2023E-02	0.1251E-02	493.54761
755.90997	0.02632	465.79880	0.2147E-02	0.1323E-02	465.35928

SLOPE	INTERCEPT
1.69607	-0.0000949

Table H
Computer Results
Light Creosote Oil Residue
Fraction 5-6

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1004.13007	0.99632	615.53479	0.1625E-02	0.9959E-03	619.46356
982.34998	0.78947	602.33563	0.1660E-02	0.1018E-02	604.15796
965.78998	0.65789	592.45319	0.1688E-02	0.1035E-02	592.58368
943.82996	0.52632	580.87054	0.1722E-02	0.1060E-02	577.31854
922.04999	0.39474	566.71185	0.1765E-02	0.1085E-02	562.27142
899.72998	0.26316	548.10413	0.1824E-02	0.1111E-02	546.94647
863.72998	0.13158	519.48401	0.1925E-02	0.1158E-02	522.42957
822.14996	0.06579	494.20117	0.2023E-02	0.1216E-02	494.41666
779.48993	0.02632	465.79880	0.2147E-02	0.1283E-02	466.00946

SLOPE	INTERCEPT
1.85217	-0.0002303

Table I
Computer Results
Light Creosote Oil Residue
Fraction 7-8

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1025.18994	0.99013	615.17267	0.1626E-02	0.9754E-03	610.657
1012.04999	0.78947	602.33563	0.1660E-02	0.9881E-03	601.969
999.44995	0.65789	592.45319	0.1688E-02	0.1001E-02	593.662
981.63007	0.52632	580.87054	0.1722E-02	0.1019E-02	581.951
960.03003	0.39474	566.71185	0.1765E-02	0.1042E-02	567.817
931.58997	0.26316	548.10413	0.1824E-02	0.1073E-02	549.308
889.28998	0.13158	519.48401	0.1925E-02	0.1124E-02	521.987
842.13000	0.06579	494.20117	0.2023E-02	0.1187E-02	491.818
800.90997	0.02632	465.79880	0.2147E-02	0.1249E-02	465.696

SLOPE	INTERCEPT
1.86616	-0.0001827

Table J
Computer Results
Light Creosote Oil Residue
Fraction 9-10

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1072.53003	0.99829	615.64996	0.1624E-02	0.9324E-03	620.10303
1053.63000	0.78947	602.33563	0.1660E-02	0.9491E-03	607.03680
1035.27002	0.65789	592.45319	0.1688E-02	0.9659E-03	594.43152
1011.33002	0.52632	580.87054	0.1722E-02	0.9888E-03	578.12335
985.23004	0.39474	566.71185	0.1765E-02	0.1015E-02	560.50702
957.14996	0.26316	548.10413	0.1824E-02	0.1045E-02	541.74164
926.72992	0.13158	519.48401	0.1925E-02	0.1079E-02	521.62823
883.71002	0.06579	494.20117	0.2023E-02	0.1132E-02	493.56015
845.18994	0.02632	465.79880	0.2147E-02	0.1183E-02	468.79446

SLOPE	INTERCEPT
2.07541	-0.0003224

Table K
Computer Results
Light Creosote Oil Residue
Fraction 11-14

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1107.80994	0.99711	615.58087	0.1624E-02	0.9027E-03	616.52661
1084.58997	0.78947	602.33563	0.1660E-02	0.9220E-03	602.58160
1067.67004	0.65789	592.45319	0.1688E-02	0.9366E-03	592.44983
1049.84998	0.52632	580.87054	0.1722E-02	0.9525E-03	581.80603
1022.48993	0.39474	566.71185	0.1765E-02	0.9780E-03	565.51776
988.10999	0.26316	548.10413	0.1824E-02	0.1012E-02	545.14178
947.78998	0.13158	519.48401	0.1925E-02	0.1055E-02	521.37433
901.71002	0.06579	494.20117	0.2023E-02	0.1109E-02	494.38040

SLOPE	INTERCEPT
1.94232	-0.0001313

Table L
Computer Results
Light Creosote Oil Residue
Fraction 15-16

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1135.70996	0.99750	615.60388	0.1624E-02	0.8805E-03	616.05322
1120.22998	0.78947	602.33563	0.1660E-02	0.8927E-03	607.02246
1093.41003	0.65789	592.45319	0.1688E-02	0.9146E-03	591.42072
1074.15002	0.52632	580.87054	0.1722E-02	0.9310E-03	580.25140
1046.25000	0.39474	566.71185	0.1765E-02	0.9558E-03	564.12274
1010.60999	0.26316	548.10413	0.1824E-02	0.9895E-03	543.60724
972.98993	0.13158	519.48401	0.1925E-02	0.1028E-02	522.05780
926.01001	0.06579	494.20117	0.2023E-02	0.1080E-02	495.29825

SLOPE	INTERCEPT
1.98475	-0.0001243

Table M
Computer Results
Light Creosote Oil Residue
Fraction 17-18-19--Dummy Fraction (Omit)

TEMP	VPRESS	T6	Y(I)	X(I)	T6CAL
1138.41003	0.65789	592.45319	0.1688E-02	0.8784E-03	589.48529
1114.65002	0.52632	580.87054	0.1722E-02	0.8971E-03	578.97632
1084.41003	0.39474	566.71185	0.1765E-02	0.9222E-03	565.50641
1050.03003	0.26316	548.10413	0.1824E-02	0.9524E-03	550.06177
912.33002	0.13158	519.48401	0.1925E-02	0.1096E-02	486.77185
960.21002	0.06579	494.20771	0.2023E-02	0.1041E-02	509.04245
906.92999	0.02632	465.79880	0.2147E-02	0.1103E-02	484.24210

SLOPE	INTERCEPT
1.64444	0.0002519

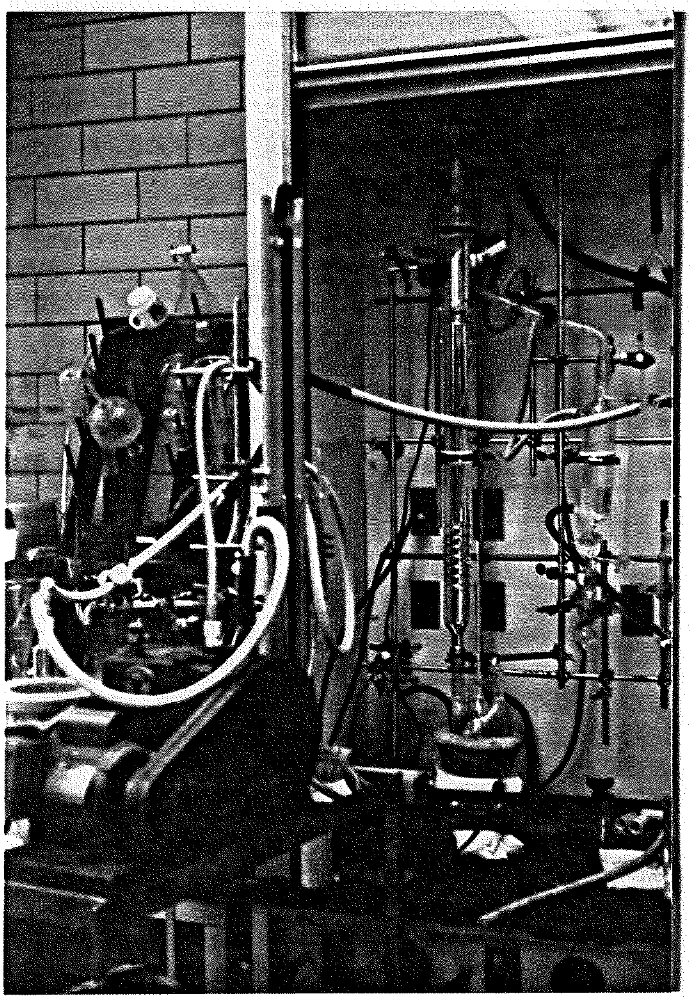
```
 $ TYPE J8R.FOR
       PROGRAM J8R
 C
 C     J=# OF COMPONENTS OF INTEREST
 C     N=# OF DATA POINTS
 C
 C     SET NTEST=1 TO BYPASS CORRECTION FACTOR ON B(I);OTHERWISE, LEAVE BLANK
 C
 C
 C     NTEMP=1 FOR OBSERVED BOILING TEMPERATURE (F)
 C     NTEMP=2 FOR OBSERVED BOILING TEMPERATURE (R)
 C     NTEMP=3 FOR OBSERVED BOILING TEMPERATURE (C)
 C     NTEMP=4 FOR OBSERVED BOILING TEMPERATURE (K)
 C
 C     NPRES=1 FOR PRESSURE IN ATM.
 C     NPRES=2 FOR PRESSURE IN MMHG.
 C     NPRES=3 FOR PRESSURE IN PSIA.
 C     NPRES=4 FOR PRESSURE IN BARS.
 C     NPRES=5 FOR PRESSURE IN KPA.
 C
 C*****MAIN PROGRAM*****
 C
       DIMENSION P(30),B(30),C(30),D(30),ZN(20),TBF(30),DIFF(30),CDEN(30)
      1,A(30),BOILNO(30),DIFF2(30),EFK(30),DZNO(30),ICOMP(80)
       READ(2,*) J
       DO 2250 K=1,J
       READ(2,25) ICOMP
       READ(2,*) N,NTEMP,NPRES
       READ(2,*) (C(I),P(I),I=1,N)
       READ(2,*) CDEN(K),TBF(K),NTEST
 C*****TEST FOR UNITS ON INPUT TEMPERATURE*****
  1100 DO 3510 I=1,N
       IF(NTEMP.EQ.1) GO TO 1001
       IF(NTEMP.EQ.2) GO TO 1002
       IF(NTEMP.EQ.3) GO TO 1003
       IF(NTEMP.EQ.4) GO TO 1004
  1002 C(I)=C(I)-459.67
       GO TO 1001
  1003 C(I)=(C(I)*1.8)+32.0
       GO TO 1001
  1004 C(I)=(C(I)*1.8)-459.67
       GO TO 1001
  1001 CONTINUE
 C*****TEST FOR UNITS ON INPUT PRESSURE*****
       IF(NPRES.EQ.1) GO TO 2001
       IF(NPRES.EQ.2) GO TO 2002
       IF(NPRES.EQ.3) GO TO 2003
       IF(NPRES.EQ.4) GO TO 2004
       IF(NPRES.EQ.5) GO TO 2005
  2002 P(I)=P(I)/760.
       GO TO 2001
  2003 P(I)=P(I)/14.69
       GO TO 2001
  2004 P(I)=P(I)*0.9869233
       GO TO 2001
  2005 P(I)=P(I)*0.009869233
       GO TO 2001
  2001 CONTINUE
       TBF(I)=(TBF(I)*1.8)+32.0
  1102 RTB=TBF(I)+459.67
       D(I)=(RTB**0.333)/CDEN(I)
  1300 IF(P(I)-.00224)1400,1400,1600
  1400 A(I)=(4.741-(ALOG(P(I))/2.30259))/(2876.663-(43.00*(ALOG(P(I))/
      #2.30259)))-.0002867
  1500 GOTO 2000
```

```
1600 IF(P(I)-1.)1700,1700,1900
1700 A(I)=(3.877-(ALOG(P(I))/2.30259))/(2387.262-(95.76*(ALOG(P(I))/
    #2.30259)))-.0002867
1800 GOTO 2000
1900 A(I)=(4.326-(ALOG(P(I))/2.30259))/(2666.376-(36.*ALOG(P(I))/
    #2.30259))-.0002867
2000 IF(B(I)-0.)2250,2100,2250
2100 BOILNO(I)=748.1*A(I)/((1./(C(I)+459.68))-.0002867+(.2145*A(I)))
     DZNO(I)=BOILNO(I)-459.68
2110 IF (BOILNO(I)-859.68)2120,2200,2200
2120 IF (BOILNO(I)-659.68)2130,2130,2150
2130 B(I)=BOILNO(I)-459.68
2140 GO TO 3510
2150 B(I)=BOILNO(I)-459.68
     EFK(I)=0.005*B(I)-1.
     IF(NTEST.EQ.1) GO TO 2210
2160 B(I)=B(I)-((2.5*(D(I)-12.0)*(ALOG(1./P(I))/2.30259))*EFK(I))
     GOTO 3510
2200 B(I)=BOILNO(I)-459.68-(2.5*(D(I)-12.0)*(ALOG(1./P(I))/2.30259))
2210 GO TO 3510
3510 CONTINUE
     DO 3800 I=1,N
     DIFF(I)=(TBF(I)-B(I))
     DIFF2(I)=(TBF(I)-DZNO(I))
3800 CONTINUE
     WRITE(3,26) ICOMP
     WRITE (3,4000)
4000 FORMAT(//,4X,'PRESS(ATM)',10X,'TEMP(F)',10X,'TBF',10X,'CALTB(F)',
    $10X,'DIFF',14X,'UOPK',10X,'A(I)',12X,'BOILNO(R)')
     WRITE(3,4001) (P(I),C(I),TBF(I),B(I),DIFF(I),D(I),A(I),BOILNO(I),
    1I=1,N)
4001 FORMAT(/,4X,F10.5,6X,F10.2,6X,F10.2,6X,F10.2,6X,F10.2,6X,F10.2
    1,6X,F10.6,6X,F10.2)
     WRITE(3,4002)
4002 FORMAT(///,7X,'EFK',17X,'DIFF2',20X,'DZNO(F)')
     WRITE(3,4003) (EFK(I),DIFF2(I),DZNO(I),I=1,N)
4003 FORMAT(/,4X,F10.8,10X,F10.2,15X,F10.2)
  25 FORMAT(80A1)
  26 FORMAT(1H1,80A1,///)
2250 CONTINUE
     ENDFILE 3
     STOP
     END
```

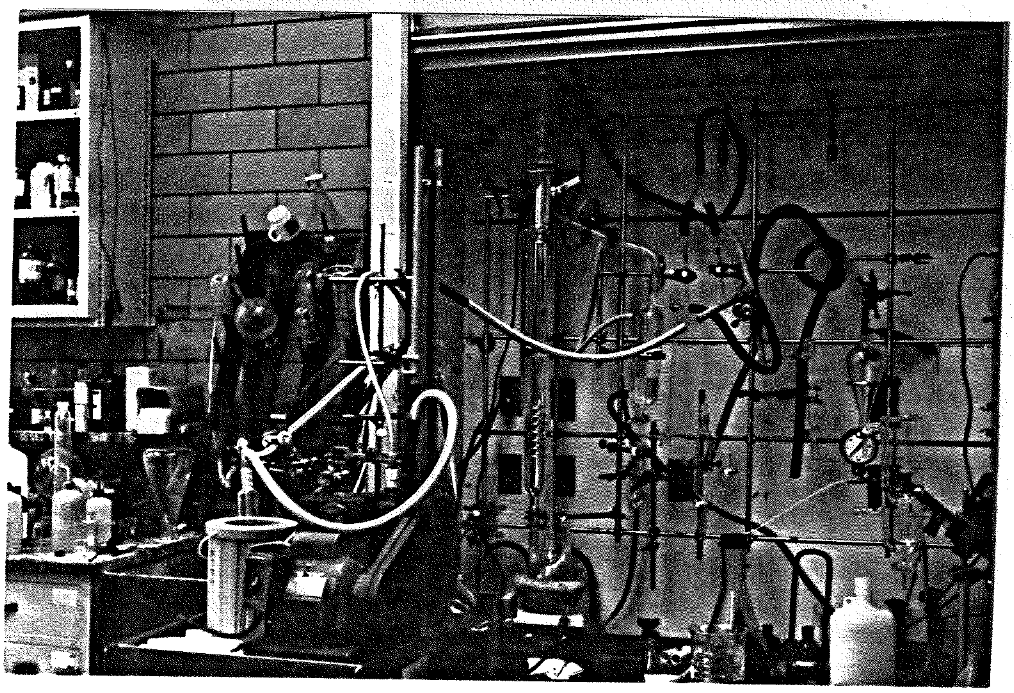
```
$ TYPE J9.FOR
      PROGRAM J9
C
C     J=# OF COMPONENTS OF INTEREST
C     N=# OF DATA POINTS
C     SET NTEMP=1 FOR TEMPERATURE IN DEGREES (F)
C     SET NTEMP=2 FOR TEMPERATURE IN DEGREES (R)
C     SET NTEMP=3 FOR TEMPERATURE IN DEGREES (C)
C     SET NTEMP=4 FOR TEMPERATURE IN DEGREES (K)
C     SET NPRES=1 FOR PRESSURE IN ATM.
C     SET NPRES=2 FOR PRESSURE IN MMHG.
C     SET NPRES=3 FOR PRESSURE IN PSIA.
C     SET NPRES=4 FOR PRESSURE IN BARS.
C     SET NPRES=5 FOR PRESSURE IN KPA.
C
C*****MAIN PROGRAM*****
C
      DIMENSION P(50),T(50),A(50),Y(50),X(50),AINT(10)
     1,SLOPE(10),ICOMP(80),YCAL(50),TCAL(50)
      READ(2,*) J
      DO 400 K=1,J
   20 READ(2,25) ICOMP
   50 READ(2,*) N,NTEMP,NPRES
      READ(2,*) (T(I),P(I),I=1,N)
  500 DO 3000 I=1,N
C*****TEST FOR UNITS ON INPUT TEMPERATURE*****
      IF(NTEMP.EQ.1) GO TO 1001
      IF(NTEMP.EQ.2) GO TO 1002
      IF(NTEMP.EQ.3) GO TO 1003
      IF(NTEMP.EQ.4) GO TO 1004
 1001 T(I)=T(I)+459.67
      GO TO 1002
 1003 T(I)=(T(I)+273.15)*1.8
      GO TO 1002
 1004 T(I)=T(I)*1.8
      GO TO 1002
 1002 CONTINUE
C*****TEST FOR UNITS ON INPUT PRESSURE*****
      IF(NPRES.EQ.1) GO TO 2001
      IF(NPRES.EQ.2) GO TO 2002
      IF(NPRES.EQ.3) GO TO 2003
      IF(NPRES.EQ.4) GO TO 2004
      IF(NPRES.EQ.5) GO TO 2005
 2002 P(I)=P(I)/760.
      GO TO 2001
 2003 P(I)=P(I)/14.69
      GO TO 2001
 2004 P(I)=P(I)*0.9869233
      GO TO 2001
 2005 P(I)=P(I)*0.009869233
      GO TO 2001
 2001 CONTINUE
      IF(P(I)-.06579)1400,1500,1500
 1400 A(1)=43.-(2672.8/(ALOG10(P(I))-4.7419))
      GO TO 3000
 1500 IF(P(I)-1.0)1600,1600,1700
 1600 A(I)=95.76-(2016.0/(ALOG10(P(I))-3.877))
      GO TO 3000
 1700 A(I)=36.00-(2510.64/(ALOG10(P(I))-4.326))
 3000 CONTINUE
C*****DO LOOP FOR CALCULATING THE COORDINATES OF THE X-Y PLOT*****
      DO 3500 I=1,N
      Y(I)=1./A(I)
      X(I)=1./T(I)
 3500 CONTINUE
```

```
C*****LEAST SQUARES ANALYSIS OF DATA*****
      SUMX=0.0
      SUMX2=0.0
      SUMXY=0.0
      SUMY=0.0
C*****CALCULATION OF THE SUMS FOR LEAST SQUARES*****
      DO 300 I=1,N
      SUMX=SUMX+X(I)
      SUMX2=SUMX2+(X(I)**2.)
      SUMXY=SUMXY+(X(I)*Y(I))
      SUMY=SUMY+Y(I)
  300 CONTINUE
C*****CALCULATION OF SLOPE AND INTERCEPT*****
      DELTAY=((SUMY/N)-(SUMXY/SUMX))
      DELTAX=((SUMX/N)-(SUMX2/SUMX))
      SLOPE(K)=DELTAY/DELTAX
      AINT(K)=(SUMY/N)-((SUMX/N)*SLOPE(K))
      DO 700 I=1,N
      YCAL(I)=AINT(K)+(SLOPE(K)/T(I))
  700 TCAL(I)=1./YCAL(I)
C*****INDIVIDUAL COMPONENT OUTPUT WRITE STATEMENTS*****
      WRITE(3,26) ICOMP
  600 WRITE(3.4000)
      WRITE(3,4500) (T(I),P(I),A(I),Y(I),X(I),TCAL(I),I=1,N)
      WRITE(3.4002)
      WRITE(3,4600) SLOPE(K),AINT(K)
  400 CONTINUE
C*****FORMAT STATEMENTS FOR COMPUTER OUTPUT*****
   25 FORMAT(80A1)
   26 FORMAT(1H1,80A1,///)
 4000 FORMAT(//,8X,'TEMP',15X,'VPRESS',15X,'T6',18X.'Y(I)',
     @16X,'X(I)',16X,'T6CAL')
 4500 FORMAT(/,4X,F10.5,10X,F10.5,10X,F10.5,10X,E10.4,10X,E10.4
     #,10X,F10.5)
 4002 FORMAT(//,8X,'SLOPE',12X,'INTERCEPT')
 4600 FORMAT(/,4X,E10.5,10X,E10.7)
      ENDFILE 3
      STOP
      END
```

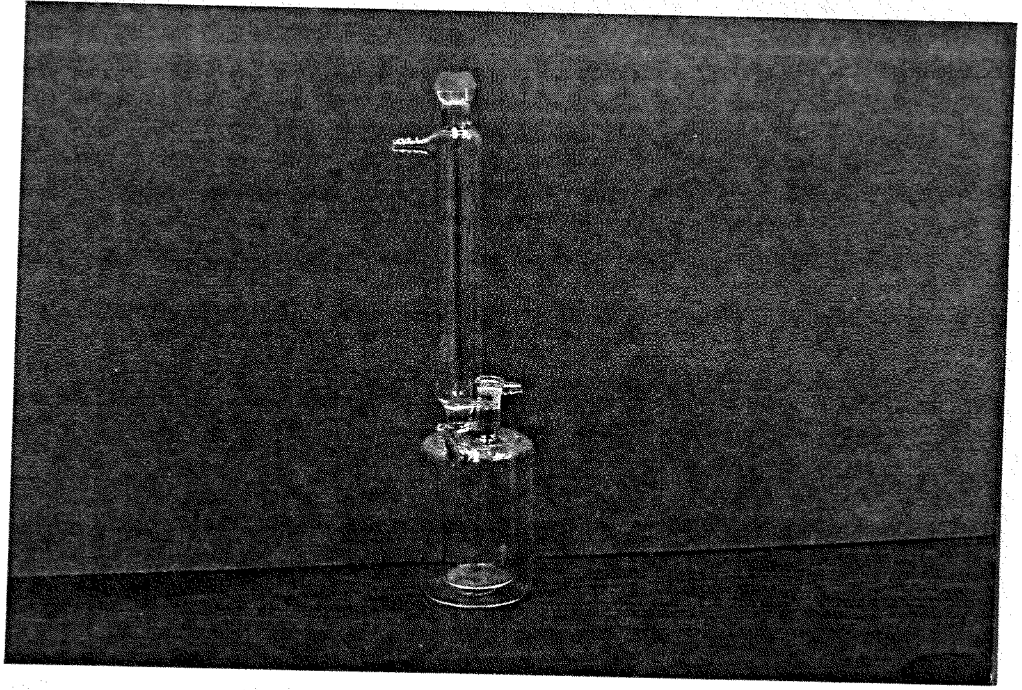
APPENDIX 4

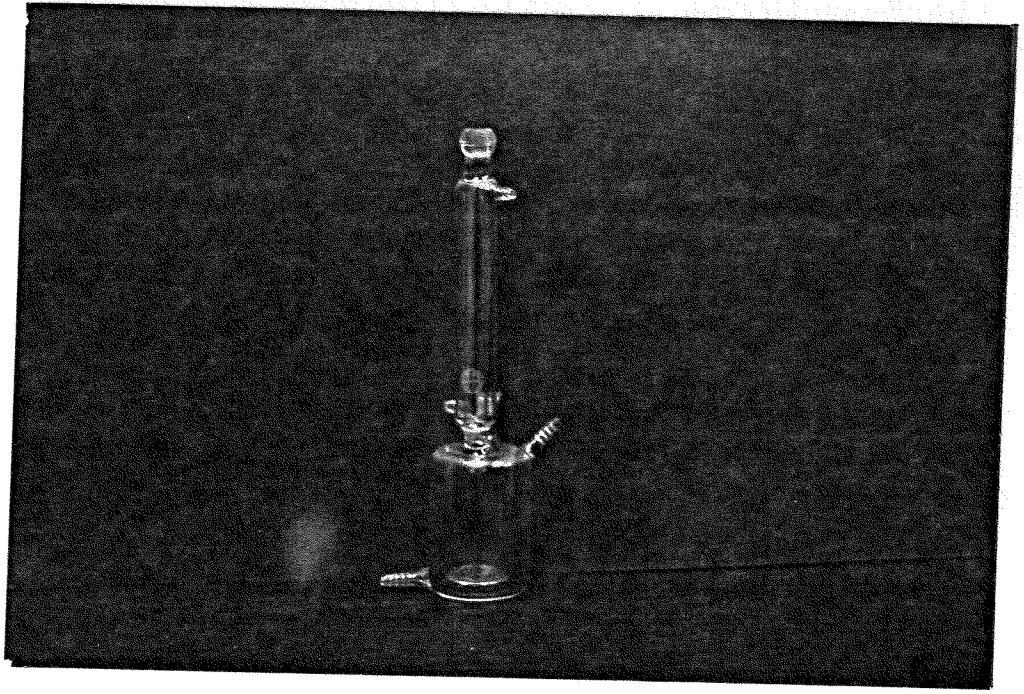


Distillation
Set
Up



Vapor Pressure Still





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