

THE UNIVERSITY OF CALGARY

MODIFIED SHAPE FACTORS FOR IMPROVED
VISCOSITY PREDICTIONS USING
CORRESPONDING STATES

by

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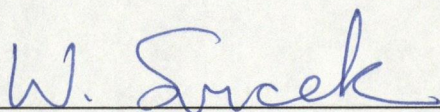
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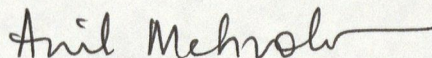
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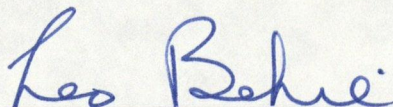
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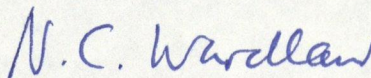
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ABSTRACT

The Ely and Hanley extended corresponding states viscosity prediction method was modified to improve the predicted liquid viscosities of pure component hydrocarbons. The procedure for determining the shape factors and the shape factor correlations have been modified. These modifications involved calculating the shape factors by inputting experimental viscosities into the method and then modelling the resulting shape factors as a function of reduced temperature. The constants in the correlation for the shape factor θ were generalized for each hydrocarbon family as a function of normal boiling point. The method was also simplified by incorporating propane as the reference fluid and substituting the COSTALD method for the complex equation of state to calculate the reference fluid density.

The predicted viscosity results from the modified method were compared with experimental data for forty six common hydrocarbons. The average absolute deviation between the predicted and experimental values for these compounds is typically within 6% for the generalized shape factor constants and within 2% for the regressed constants. The predicted viscosities are generally one order of magnitude better than those from the TRAPP program, especially for olefins and naphthenic compounds.

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NOMENCLATURE

$A_{vp}, B_{vp}, C_{vp}, D_{vp}$	vapor pressure constants
f	equivalent substance temperature reducing ratio
h	equivalent substance volume reducing ratio
M	molecular weight, g/mol
P	absolute pressure, kPa
P_c	critical pressure, kPa or atm.
P_v	vapor pressure, kPa
T	absolute temperature, K
T_b	normal boiling point, K
T_c	critical temperature, K
T_r	reduced temperature
V	molar volume, cm^3/mol
V_c	critical volume, cm^3/mol
$V_r^{(0)}$	corresponding states function for normal fluids for COSTALD method
$V_r^{(\delta)}$	deviation function for COSTALD method
V_s	saturated liquid volume, L/mol
V^*	characteristic volume for COSTALD method, L/mol
x	mole fractions
Z	compressibility factor
Z_c	critical compressibility factor
$a, b, c, \dots, A, B, C, \dots$	constants

Greek Letters

η	dynamic viscosity, mPa-s
η_c	critical viscosity, mPa-s
$\eta^{(1)}, \eta^{(2)}, \Delta\eta$	reference fluid viscosity correlations
σ	effective molecular diameter
ε	intermolecular potential energy well
ρ	density, g/cm ³
ρ_c	critical density, g/cm ³
θ	energy shape factor
ϕ	size shape factor
ω	acentric factor
γ	constant

Subscripts

i, j	components
SRK	Soave Redlich Kwong
o	reference fluid
i	fluid of interest

Abbreviations

COSTALD	Corresponding States Liquid Density
TRAPP	Transport Properties Prediction computer program

CHAPTER 1

INTRODUCTION

1.1 General Introduction

In the petroleum industry, viscosity of crude oils and natural gas is an important parameter in pressure drop calculations for piping systems, surface facilities and flow through porous media. With the increased popularity of process and reservoir simulators, there is a need for a reliable and accurate analytical predictive method for liquid hydrocarbon viscosity calculations.

Several methods for the prediction of viscosity are available in the literature (Reid et al, 1986, API, 1987). Gas phase viscosity is primarily a function of momentum transfer by collisions between molecules and is adequately described by kinetic theory. In liquids, however, the transfer of momentum is dominated by interacting force fields between the densely packed molecules because the molecular separation distance falls within the effective field of these forces. For calculating liquid phase viscosity, there is no simple theoretical method of calculation and many of the available methods are either empirical in nature or derived from corresponding states theory (Reid et al, 1986). Most of the empirical methods are applicable over limited ranges of temperature and pressure and invariably require a certain amount of viscosity data as input. Conversely, the corresponding states methods are predictive and can be applied over a wide range of temperature and pressure. Unfortunately, current

corresponding states models fail to consistently predict the viscosity of most non-paraffinic hydrocarbons unless a similar non-paraffinic reference fluid is used (Ely and Hanley, 1981, Teja and Rice, 1981).

1.2 Research Objective

In order to predict the viscosity of a mixture, it is essential that viscosity of the pure components which make up the mixture be accurately predicted. Only then, can the method and the mixing rules be evaluated for predicting the properties of a mixture. Therefore, the primary objective of this research is to modify the existing shape factors in the extended corresponding states method to improve the viscosity predictions for pure component liquid hydrocarbons. The key to the extended corresponding states method providing an accurate viscosity prediction for a wide variety of compounds is to obtain the correct magnitude of the shape factors, the variation of these shape factors with temperature and the proper functional form to fit this variation. A secondary objective of the research is to simplify the method.

CHAPTER 2

LITERATURE REVIEW

The viscosity of hydrocarbons has been discussed in numerous studies. Due to the extensive number of these studies, this review is confined to calculation methods based on the principle of corresponding states.

In 1969, Tham and Gubbins presented a corresponding states method derived from statistical mechanics under well defined assumptions to predict the transport properties of pure monatomic dense fluids. This work was subsequently expanded to polyatomic dense fluids based on extending the two parameter corresponding states with a third parameter to account for hindered rotation of such fluids (Tham and Gubbins, 1970). This work was further expanded to predict the transport properties of mixtures by Mo and Gubbins (1974). They stated that in addition to mixing rules for the corresponding states parameters, a mass mixing rule was required for transport properties. Under well defined assumptions, a set of mixing rules were derived. The resulting mixing rules for the corresponding states parameters were identical to the van der Waals one fluid approximation.

In 1976, Hanley developed an extended corresponding states method to calculate transport properties of mixtures based on the shape factor approach developed by Leach (1967). Transport properties of any fluid or mixture could be determined from the properties of a reference

fluid, which was chosen to be methane. The reference fluid viscosity was correlated as a function of temperature and density (Hanley, McCarty and Haynes, 1975). To calculate the density of methane, the equation of state of Goodwin (1974) was used. Since no viscosity data was required as input, the method can be classed as purely predictive. The mixing rules for the method were those of Mo and Gubbins (1974). For fluids which do not correspond with the reference fluid, Hanley (1976) derived a correction factor based on so called modified Enskog theory.

In 1981, Ely and Hanley slightly modified the method of Hanley. They reported that the major difficulty of using methane as a reference fluid was the freezing of methane at a reduced temperature of 0.48, which is above the reduced temperatures encountered for other liquid hydrocarbons. The difficulty in extrapolating the methane viscosity to high reduced densities and the non-correspondence of methane with several other hydrocarbons at high reduced densities posed additional problems. To overcome these difficulties, an extended equation of state and modified viscosity correlation were developed. The form of the equation of state was a 32 term BWR-type proposed by Jacobsen and Stewart (1973). The non-correspondence correction factor and high density term were modified in the viscosity correlation. Ely and Hanley used the mixing rules of Mo and Gubbins (1974) for the corresponding states parameters but derived a different mass mixing rule based on the radial distribution function. Although modified, the method was still based on the extension of the corresponding states

method by molecular shape factors developed by Leach (1967). The shape factors were derived from light paraffinic substances for the most part, resulting in significant errors when these were used to predict the viscosity of naphthenic and some aromatic compounds (Ely and Hanley, 1981).

Recently at the University of Calgary, Johnson et al (1987) presented a method based on the extended principle of corresponding states for the prediction of Athabasca bitumen viscosity. Heavy hydrocarbons such as bitumen contain cyclic and aromatic compounds and due to the inherent limitations in the derivation of the shape factors, using the original correlations gave inadequate viscosity predictions. Johnson et al (1987), and Mehrotra and Svrcek (1987) showed that the shape factors in the model required modification in order to predict the density and viscosity of Alberta bitumens.

In 1984, Ely stated that the three areas where the Ely-Hanley extended corresponding states method could be improved were the reference fluid, the shape factors and the mixing rules. Ely (1984) substituted propane for methane as the reference fluid to eliminate factors to correct for the non-correspondence of methane with other fluids. This also resulted in an extended reduced temperature range due to propane having the lowest reduced triple point temperature of the normal paraffins. Slightly simplified shape factor correlations, tested with a wider variety of pure compounds, were also developed.

In 1981, Teja and Rice developed a corresponding states method for the viscosity of liquid mixtures. This method was based on the three

parameter corresponding states principle of Pitzer et al (1955), extended by the use of two non-spherical reference fluids and applied the liquid viscosity correlation of Letsou and Stiel (1973). It should be noted that this method does require the choice of two reference fluids and at least two viscosity points to correlate the viscosities of the reference fluids.

In 1980, Christensen and Fredenslund developed a corresponding states method to predict the viscosity of mixtures based on the work of Tham and Gubbins (1969, 1970, 1974). However, an analytical correlation to calculate the hindered rotation coefficient was derived. This work was later modified by Pedersen et al (1984), based on the work of Ely and Hanley (1981), to predict the viscosity of crude oils. New mixing rules and a slightly modified correlation to calculate the hindered rotation coefficient were derived.

CHAPTER 3

CORRESPONDING STATES THEORY

3.1 The Principle of Corresponding States

The principle of corresponding states is one of the most useful methods for predicting unknown properties of fluids. Simply, the principle states that dimensionless properties of two fluids have the same numerical value at the same reduced conditions (Leach, 1967). Hence, the corresponding states principle allows the prediction of unknown properties of a fluid from known properties of another fluid.

3.2 Two Parameter Corresponding States

The principle of corresponding states was originally stated by van der Waals in 1873 by writing his cubic equation of state in reduced variables (Pitzer, 1939). In 1939, Pitzer derived the principle from statistical mechanics. The derivation was based on four assumptions as summarized by Prausnitz (1969):

- (1) Classical statistical mechanics is applicable.
- (2) The potential energy between two molecules depends only on the distance between the molecules and not on their mutual orientation. That is, the potential energy force fields are assumed to be spherically symmetric.
- (3) The potential energy of a pair of molecules may be expressed as:

$$\frac{u(r)}{\varepsilon} = f\left(\frac{r}{\sigma}\right) \quad (3.1)$$

where, ε = intermolecular potential energy well

r = distance between the centers of the molecules

σ = effective molecular diameter

This equation implies that if the potential energy of any fluid is written in reduced variables, then that same function is valid for any other fluid. These fluids are said to be conformal or simple fluids.

(4) The potential energy of all molecules is the sum of the potential energies of all possible pairs of molecules.

These four assumptions are satisfied by fluids composed of simple monatomic spherically symmetric molecules (Leach et al, 1966).

If two fluids are conformal, the potential energy of any fluid, i , may be expressed in terms of another fluid, o :

$$u_i(r) = c u_o\left(\frac{r}{g}\right) \quad (3.2)$$

where c and g are conformal parameters.

$$c = \frac{\varepsilon_i}{\varepsilon_o} \quad (3.3)$$

$$g = \frac{\sigma_i}{\sigma_o} \quad (3.4)$$

The molecular parameters are difficult to obtain accurately and can be shown to be directly proportional to critical properties, with the same

proportionality constants for all fluids (Leach et al, 1968):

$$\varepsilon \propto T_c \quad (3.5)$$

$$\sigma^3 \propto V_c \quad (3.6)$$

Similarly, compressibility of any fluid, i, may be expressed in terms of a reference fluid, o :

$$z_i(T, V) = z_o \left[T \left(\frac{T_{c_o}}{T_{c_i}} \right), V \left(\frac{V_{c_o}}{V_{c_i}} \right) \right] \quad (3.7)$$

3.3 The Corresponding States Principle for Mixtures

The most useful method of extending corresponding states to mixtures has been the pseudo-critical concept. Pseudo-critical properties may be defined as the critical properties of a hypothetical pure fluid which represents a mixture when both are at the same P, V, T conditions (Leach, 1967).

An equation of state in terms of the compressibility factor may be written in terms of reduced variables:

$$z = f \left(\frac{T}{T_c}, \frac{V}{V_c} \right) = f(T_r, V_r) \quad (3.8)$$

Hence, pure fluid properties may be determined if the critical properties are known. If a mixture is represented as a pseudo pure component, the compressibility may be written similarly:

$$z_m = f\left(\frac{T}{T_{pc}}, \frac{V}{V_{pc}}\right) \quad (3.9)$$

where, T_{pc} = pseudo-critical temperature of the mixture

V_{pc} = pseudo-critical volume of the mixture

Many mixing rules have been developed for calculating pseudo-critical properties of mixtures and are summarized by Reid et al (1986).

3.4 Extension of Corresponding States to Non-Conformal Fluids and Mixtures

The theory of corresponding states was originally derived for conformal or simple fluids and mixtures comprised of such fluids, i.e., fluids with spherically symmetric potential energy force fields. The potential functions for these fluids depend only on the distance between the molecules and not on their mutual orientation. However, most fluids are non-conformal or complex and two parameter corresponding states required extension in order to accurately represent these fluids.

In one approach, the non-conformality of fluids was accounted for by introducing an empirical third parameter into the equation of state, in terms of the compressibility factor, resulting in three parameter corresponding states (Leach, 1967). Although many different parameters were proposed, the most widely accepted additional parameter is the acentric factor proposed by Pitzer. The acentric factor was to represent the non-conformality of a molecule, i.e. the non-sphericity of its potential energy field, and is related to the reduced saturation

pressure at a reduced temperature of 0.7:

$$\omega = -\log(P_r^{\text{sat}})_{T_r=0.7} - 1.0 \quad (3.10)$$

Pitzer et al (1955) extended the corresponding states principle by introducing a Taylor series expansion for the compressibility factor in ω about the point $\omega = 0$:

$$z = z|_{\omega=0} + \left. \frac{\partial z}{\partial \omega} \right|_{\omega=0} \omega + \dots \quad (3.11)$$

Equation 3.11 is usually truncated at the linear term. Pitzer et al (1955) reported that the introduction of the acentric factor as a third parameter in corresponding states decreased errors by about an order of magnitude over those obtainable with two parameter corresponding states. However, Leach (1967) showed that if three parameters were sufficient to describe the thermodynamic data of compounds, then the choice of a third parameter was arbitrary since any third parameter could be predicted in terms of another. If three parameters were not sufficient, then the choice of a third parameter was dependent on the property being predicted. Hence, corresponding states can only be improved to a certain limit by the addition of a third parameter and if greater accuracy is demanded, then it can only be achieved at the expense of additional parameters (Leach, 1967).

An alternative approach to account for the non-conformality of fluids was to modify the two parameter corresponding states

proportionality between molecular parameters and critical properties, by multiplying the critical properties by variable factors, called molecular shape factors:

$$\varepsilon \propto \theta(T)T_c \quad (3.12)$$

$$\sigma^3 \propto \phi(T)V_c \quad (3.13)$$

The proportionality constants applicable to θT_c and ϕV_c are considered to be the same for all fluids (Leach et al, 1968). This approach is known as extended corresponding states and the theoretical basis and properties of these shape factors have been discussed (Leach, 1967, Cook and Rowlinson, 1953, Gilbert, 1963). The mixing rules for pseudo critical properties of mixtures obeying two parameter corresponding states are also valid for mixtures of non-conformal fluids whose critical properties have been multiplied by molecular shape factors.

Shape factors were found to be temperature dependent and, to a limited extent, density dependent. Generally, the shape factors are density independent for gases but are density dependent for dense fluids and liquids (Leach, 1967).

Shape factors used for determining the properties of a complex fluid from known properties of a reference fluid are represented with two subscripts. The first subscript represents the particular complex fluid whose properties are to be determined and the second represents the reference fluid whose properties are known. For example, to evaluate the compressibility factor of any fluid, i , from a reference

fluid, o, Equation 3.7 is replaced with:

$$z_i(T, V) = z_o \left[T \left(\frac{T_{c_o}}{\theta_{i,o} T_{c_i}} \right), V \left(\frac{V_{c_o}}{\phi_{i,o} V_{c_i}} \right) \right] \quad (3.14)$$

Leach (1967) determined that density independent shape factors usually could not be determined which equate the configuration integrals of two complex fluids. He also determined that density dependent shape factors which equate the configuration integrals of two complex fluids would result in the compressibility factors of the two fluids not being equal at corresponding reduced conditions. However, shape factors can be determined theoretically by simultaneous solution of the conformal equations (Rowlinson and Watson, 1969):

$$A_i(T, V) = f_{i,o} A_o(T/f_{i,o}, V/h_{i,o}) - RT \ln h_{i,o} \quad (3.15)$$

$$z_i(T_i, V_i) = z_o(T/f_{i,o}, V/h_{i,o}) \quad (3.16)$$

where, A = the Helmholtz free energy

$f_{i,o}, h_{i,o}$ = reducing ratios

$$f_{i,o} = \left(\frac{T_{c_i}}{T_{c_o}} \right) \theta_{i,o} \quad (3.17)$$

$$h_{i,o} = \left(\frac{V_{c_i}}{V_{c_o}} \right) \phi_{i,o} \quad (3.18)$$

Similarly, Leach (1967) was able to define "practical" shape factors

which were derived by equating the compressibility factors and fugacity coefficients of a complex fluid and the reference fluid:

$$z_i(T, V) = z_o(T/f_{i,o}, V/h_{i,o}) \quad (3.19)$$

$$\ln\left(\frac{f_i(T, V)}{P}\right) = \ln\left(\frac{f_o(T/f_{i,o}, V/h_{i,o})}{P}\right) \quad (3.20)$$

These equations provided values of shape factors especially accurate for vapor-liquid equilibrium calculations. Leach (1967) determined the shape factors for paraffins up to n-pentadecane (C_{15}) using methane as a reference fluid and fitted the results to two empirical correlations.

3.5 Viscosity Prediction by the Ely-Hanley Extended Corresponding States Method

The reduced viscosity may be expressed as:

$$\eta_r = \frac{\eta}{\eta_c} = f(T_r, \rho_r) \quad (3.21)$$

The critical viscosity, η_c , is defined from kinetic theory as:

$$\eta_c = \text{const.} \frac{M^{1/2} T_c^{1/2}}{V_c^{2/3}} \quad (3.22)$$

According to corresponding states, the function f is the same for all

conformal fluids. Hence, viscosity of any fluid may be expressed in terms of a reference fluid, much the same as the compressibility factor. As previously shown, in two parameter corresponding states, fluids are characterized by an energy parameter, ϵ , and a distance parameter, σ . According to Hanley (1976), viscosity of any fluid, i , can be expressed in terms of a reference fluid, o :

$$\eta_i(\rho, T) = \eta_o \left[\rho \left(\frac{\sigma_i}{\sigma_o} \right)^3, T \left(\frac{\epsilon_o}{\epsilon_i} \right) \right] \left(\frac{M_i}{M_o} \right)^{1/2} \left(\frac{\sigma_o}{\sigma_i} \right)^2 \left(\frac{\epsilon_i}{\epsilon_o} \right)^{1/2} \quad (3.23)$$

Since $\epsilon/k \propto T_c$ and $\sigma^3 \propto \rho_c$, this expression may be rewritten:

$$\eta_i(\rho, T) = \eta_o \left[\rho \left(\frac{\rho_{co}}{\rho_{ci}} \right), T \left(\frac{T_{co}}{T_{ci}} \right) \right] \left(\frac{M_i}{M_o} \right)^{1/2} \left(\frac{\rho_{ci}}{\rho_{co}} \right)^{2/3} \left(\frac{T_{ci}}{T_{co}} \right)^{1/2} \quad (3.24)$$

These expressions, however, only hold true for conformal fluids. For non-conformal fluids, the extended corresponding states method can be used, where shape factors θ and ϕ are introduced to account for the non-conformality of the molecules. Introducing the reducing ratios defined by Equations 3.17 and 3.18 into Equation 3.24, the expression for viscosity can be rewritten for non-conformal fluids as:

$$\eta_i(\rho, T) = \eta_o \left[\rho h_{i,o}, T/f_{i,o} \right] \left(\frac{M_i}{M_o} \right)^{1/2} h_{i,o}^{-2/3} f_{i,o}^{1/2} \quad (3.25)$$

This may be rewritten as Equation 3.26:

$$\eta_i(\rho, T) = \eta_o(\rho_o, T_o) \left(\frac{M_i}{M_o} \right)^{1/2} h_{i,o}^{-2/3} f_{i,o}^{1/2} \quad (3.26)$$

$$\text{where, } \rho_o = \rho h_{i,o} \quad (3.27)$$

$$T_o = T/f_{i,o} \quad (3.28)$$

When determining properties by corresponding states, the reference fluid should be as similar as possible to the complex fluid whose properties are to be determined. Ely and Hanley (1981) had used methane as a reference fluid for earlier work because they had been concerned with the properties of LNG. However, concerned with studying heavier hydrocarbons, they sought a more appropriate reference fluid. Unfortunately, at that time, methane was the only fluid with sufficient and reliably correlated viscosity and P,V,T data, so it was used again as the reference fluid. In practice, one problem they observed with the use of methane as a reference fluid was that it freezes at a reduced temperature of 0.48, which is above reduced temperatures encountered for other hydrocarbons in the liquid phase. This problem was overcome by constructing a 32 term BWR-type extended methane equation of state for P,V,T calculations (Ely and Hanley, 1981). For viscosity, it was not possible to simply extrapolate the methane viscosity surface to high values of the reduced density. Therefore, Ely and Hanley (1981) attempted to calculate pseudo methane viscosities via extended corresponding states and then fit the real and pseudo

viscosity values to the reference fluid viscosity correlation. From this, they observed a non-correspondence of methane with other paraffins at these high reduced densities. To overcome this problem, they modified the non-correspondence factor originally proposed by Hanley (1976) and then fit the pseudo viscosities to the high density term of the reference fluid viscosity correlation.

Recently, as sufficient reliable viscosity and P,V,T data became available, Ely (1984) substituted propane for methane as the reference fluid. This was based on the observations that (a)propane has the lowest reduced triple point temperature and(b)the non-correspondence of propane with methane was the same as that of eicosane and methane. This indicated correspondence and eliminated the need for empirical corrections as well as resulting in a wider reduced temperature range.

The equation of state for calculation of the reference fluid equivalent density and the reference fluid viscosity correlation are shown in Tables 1 and 2, respectively. The forms of these equations are the same for both the propane and methane reference fluids.

The shape factors θ and ϕ were originally calculated by equations of the form developed by Leach (1967):

$$\theta_{i,o} = 1 + (\omega_i - \omega_o)(a_1 + b_1 \ln T_i^+ + (c_1 + d_1/T_i^+)(V_i^+ - 0.5)) \quad (3.29)$$

$$\phi_{i,o} = [1 + (\omega_i - \omega_o)(a_2(V_i^+ + b_2) + c_2(V_i^+ + d_2) \ln T_i^+)] \frac{z_{co}}{z_{ci}} \quad (3.30)$$

Table 1
Reference Fluid Equation of State*

$$P = \sum_{n=1}^9 a_n(T) \rho^n + \exp(-\gamma \rho^2) \sum_{n=10}^{15} a_n(T) \rho^{2n-17}$$

$a_1 = RT$	$a_9 = b_{19}/T^2$
$a_2 = b_1 T + b_2 T^{1/2} + b_3 + b_4 + b_5/T^2$	$a_{10} = b_{20}/T^2 + b_{21}/T^3$
$a_3 = b_6 T + b_7 + b_8/T + b_9/T^2$	$a_{11} = b_{22}/T^2 + b_{23}/T^4$
$a_4 = b_{10} T + b_{11} + b_{12}/T$	$a_{12} = b_{24}/T^2 + b_{25}/T^3$
$a_5 = b_{13}$	$a_{13} = b_{26}/T^2 + b_{27}/T^4$
$a_6 = b_{14}/T + b_{15}/T^2$	$a_{14} = b_{28}/T^2 + b_{29}/T^3$
$a_7 = b_{16}/T$	$a_{15} = b_{30}/T^2 + b_{31}/T^3 + b_{32}/T^4$
$a_8 = b_{17}/T + b_{18}/T^2$	

* numerical values of constants are given in Ely and Hanley (1981) and Ely (1984)

Table 2
Reference Fluid Viscosity Correlation*

$$\eta(\rho, T) = \eta^{(1)}(T) + \eta^{(2)}(T)\rho + \Delta\eta(\rho, T)\chi_{\eta}$$

$$\eta^{(1)} = C_{10} T^{1/2} \sum_{n=1}^9 C_n (T/b_4)^{(n-4)/3}$$

$$\eta^{(2)} = b_1 + b_2 [b_3 - \ln(T/b_4)]^2$$

$$\Delta\eta = \exp(a_1 + a_2/T) \{ \exp[(a_3 + a_4/T^{3/2})\rho^{0.1} + (\rho/\rho_c - 1)\rho^{0.5} (a_5 + a_6/T + a_7/T^2)] - 1.0 \}$$

$$\chi_{\eta} = \left(\left[1 - 1.5 \frac{T}{f_{x,o}} \left(\frac{\partial f_{x,o}}{\partial T} \right)_v \right] \frac{z_{cx}}{z_{co}} \right)^{1/2} \quad \text{for methane}$$

$$\chi_{\eta} = 1 \quad \text{for propane}$$

* numerical values of constants are given in Appendix C, Ely and Hanley (1981) and Ely (1984)

$$\text{where } T_i^+ = \min[2, \max(\text{Tr}_i, 0.5)] \quad (3.31)$$

$$V_i^+ = \min[2, \max(\text{Vr}_i, 0.5)] \quad (3.32)$$

Ely and Hanley (1981) removed the restriction imposed by Equation 3.31 on Tr_i and then redetermined the constants in Equations 3.29 and 3.30. In the most recent model developed by Ely (1984), new shape factors based on the propane reference fluid were calculated using the conformal equations with recent experimental data and more accurate equations of state. He then developed new shape factor correlations. The density terms in the shape factor correlations were found to be statistically insignificant, resulting in density independent correlations. The simplified correlations are given by Equations 3.33 and 3.34:

$$\theta_{i,0} = 1 + (\omega_i - \omega_0)(a + b \ln(\text{Tr})) \quad (3.33)$$

$$\phi_{i,0} = [1 - (\omega_i - \omega_0)(c + d \ln(\text{Tr}))] \frac{Z_c}{Z_{c0}} \quad (3.34)$$

Density of the fluid of interest is calculated after the shape factors. Because the original shape factor correlations were functions of density, calculation of the shape factors was iterative. Since the new shape factor correlations are density independent, calculation of the shape factors is non-iterative.

This method is extended to mixtures by applying the mixing rules, given in Table 3, for the reducing ratios f and h and the molecular

weight (Ely and Hanley, 1981, Ely, 1984). The calculation of viscosity by the extended corresponding states method proceeds in the following manner:

(i) Required Input:

- the number of components in the mixture and their mole fraction
- P_c , V_c , T_c , ω and M of each component in the mixture
- T and P at which the viscosity is to be calculated

(ii) Calculate:

- (1) $\phi_{i,0}$, $h_{i,0}$ (For a mixture, apply mixing rules to calculate $h_{x,0}$)
- (2) $\theta_{i,0}$, $f_{i,0}$ (For a mixture, apply mixing rules to calculate $f_{x,0}$)
- (3) M_x for a mixture
- (4) $T_o = T/f$ and $P_o = Ph/f$
- (5) ρ_o at T_o and P_o using the reference fluid equation of state.
- (6) η_o at T_o and ρ_o using the reference fluid viscosity correlation.
- (7) η

Table 3
 Mixing Rules for the Extended
 Corresponding States Viscosity Method

$$h_{x,o} = \sum_i \sum_j x_i x_j h_{ij,o}$$

$$h_{ij,o} = 1/8 (h_{i,o}^{1/3} + h_{j,o}^{1/3})^3$$

$$h_{i,o} = (V_{c_i}/V_{c_o}) \phi_{i,o}$$

$$f_{x,o} = 1/h_{x,o} \sum_i \sum_j x_i x_j f_{ij,o} h_{ij,o}$$

$$f_{ij,o} = (f_{i,o} f_{j,o})^{1/2}$$

$$f_{i,o} = (T_{c_i}/T_{c_o}) \theta_{i,o}$$

$$h_{x,o}^{4/3} f_{x,o}^{1/2} M_x^{1/2} = \sum_i \sum_j x_i x_j h_{ij,o}^{4/3} f_{ij,o}^{1/2} M_{ij}^{1/2}$$

$$M_{ij} = 2M_i M_j / (M_i + M_j)$$

CHAPTER 4

DATABASE

4.1 Experimental Viscosities

A database of experimental viscosities was assembled to provide data for modelling the modified extended corresponding states method, for testing the method and comparing it to the existing method. The database consists of forty six common hydrocarbons. Table 4 lists the included compounds and corresponding data references. These compounds were chosen for the most part because they had been used by Ely and Hanley (1981) to test their existing method. However, more cycloparaffins and aromatics were included in order to choose compounds similar to those contained in heavy oils and bitumens so that results of this research could be extended to these substances.

In general, viscosity data from various sources is significantly scattered, possibly due to using poor measurement methods and impure compounds. Unfortunately, recent accurate experimental techniques, such as the oscillating piezoelectric crystal, have not been applied to many organic liquids (Ely and Hanley, 1981). Typically, viscosity has been measured by various methods, such as the capillary tube, falling cylinder, rolling ball, and oscillating disk viscometers. Although each method has its advantages and disadvantages, the major source of error is in the calibration of the viscometer. As a result, reported experimental viscosities at corresponding conditions may agree within a

Table 4
Database Components and Viscosity Data Sources

<u>Component</u>	<u>References</u>
methane	Haynes(1973)
ethane	TRC(1986), Swift et al(1960)
propane	Diller(1982)
n-butane	TRC(1986), Lipkin et al (1942)
i-butane	TRC(1986)
n-pentane	TRC(1986), Vargaftik(1975)
i-pentane	TRC(1986)
n-hexane	TRC(1986), Vargaftik(1975)
n-heptane	TRC(1986), Vargaftik(1975)
n-octane	TRC(1986), Vargaftik(1975)
n-nonane	TRC(1986), Vargaftik(1975)
n-decane	TRC(1986), Vargaftik(1975)
n-undecane	TRC(1986)
n-dodecane	TRC(1986)
n-tridecane	TRC(1986)
n-tetradecane	TRC(1986)
n-pentadecane	TRC(1986)
n-hexadecane	TRC(1986)
n-heptadecane	TRC(1986)
n-octadecane	TRC(1986)
n-nonadecane	TRC(1986)
n-eicosane	TRC(1986)
ethene	TRC(1986)
propene	TRC(1986)
1-butene	TRC(1986)
1-pentene	TRC(1986)
1-hexene	TRC(1986)
cyclopentane	TRC(1986)
methylcyclopentane	TRC(1986)
ethylcyclopentane	TRC(1986)
n-propylcyclopentane	TRC(1986)
cyclohexane	TRC(1986)
methylcyclohexane	TRC(1986)
ethylcyclohexane	TRC(1986)
n-propylcyclohexane	TRC(1986)
n-butylcyclohexane	TRC(1986)
benzene	TRC(1986), Medani and Hasan(1977)
toluene	TRC(1986), Medani and Hasan(1977)
ethylbenzene	TRC(1986)
o-xylene	TRC(1986)
m-xylene	TRC(1986)
p-xylene	TRC(1986)
n-propylbenzene	TRC(1986)
isopropylbenzene	TRC(1986)
n-butylbenzene	TRC(1986)
naphthalene	Evans(1938), Grunberg-Nissan(1951)

few percent or deviate substantially from one another. For example, for propane Diller (1982) compared previous measurements to his oscillating piezoelectric crystal measurements. He reported that the capillary tube measurements of Gerf and Galkov (1940) deviated by about 2% but the falling cylinder measurements of Swift et al (1959) deviated by as much as 12% .

Most of the viscosity data used in the database were obtained from the Thermodynamics Research Center (TRC) Data Book (1986). For the most part, these data were based on the same sources as those recommended by Ely and Hanley (1981). These data were chosen because Ely and Hanley had analyzed their data for consistency and the TRC had smoothed their data. Using these data would also make comparisons between the modified and existing methods fair. Errors for these data are believed to be in the order of 5% to 15% (Ely and Hanley, 1981). Although most of the selected data were previously screened, all sources of data for each component were plotted against temperature to ensure consistency.

If the TRC data were based on entirely different sources than those recommended by Ely and Hanley, then the two sources were compared. In many cases, the data compiled by Vargaftik (1975) were also compared. Typically, scatter was within 5%, so the TRC data were also used in this case. If the compound was not tested by Ely and Hanley, then the TRC (1986), Vargaftik (1975) and data compiled by Grunberg and Nissan (1951) were compared. Since scatter between these data was negligible, the TRC data were used in this case also.

However, the TRC data was only reported to the normal boiling point. Above the normal boiling point data are very limited, so any data recommended by Ely and Hanley or the data of Vargaftik were used.

For example, the data used for n-pentane is presented in Table 5 and plotted on Figure 1. The TRC data for n-pentane were from entirely different sources than those recommended by Ely and Hanley. It can be seen that the data are not very scattered. This reflects the previous screening of the data, and so the TRC data was incorporated into the database. The data for all the compounds in the database, except methane and propane, were selected in a similar manner. The data for methane and propane were taken from oscillating piezoelectric crystal measurements reported by the National Bureau of Standards in the United States (Haynes, 1973, Diller, 1982). Data for all compounds are summarized in Appendix A.

All of the data in the database were compiled, checked for consistency and then incorporated into the database over a period of two months. However, the data available in the literature has large gaps. There is very little reliable published data, especially at temperatures above the normal boiling point. This data needs to be experimentally determined or obtained from unpublished sources, if possible, such as the National Bureau of Standards (NBS) in the United States, the DECHEMA viscosity database, the AIChE Dippr database or company files.

Table 5
n-Pentane Experimental Viscosity Data

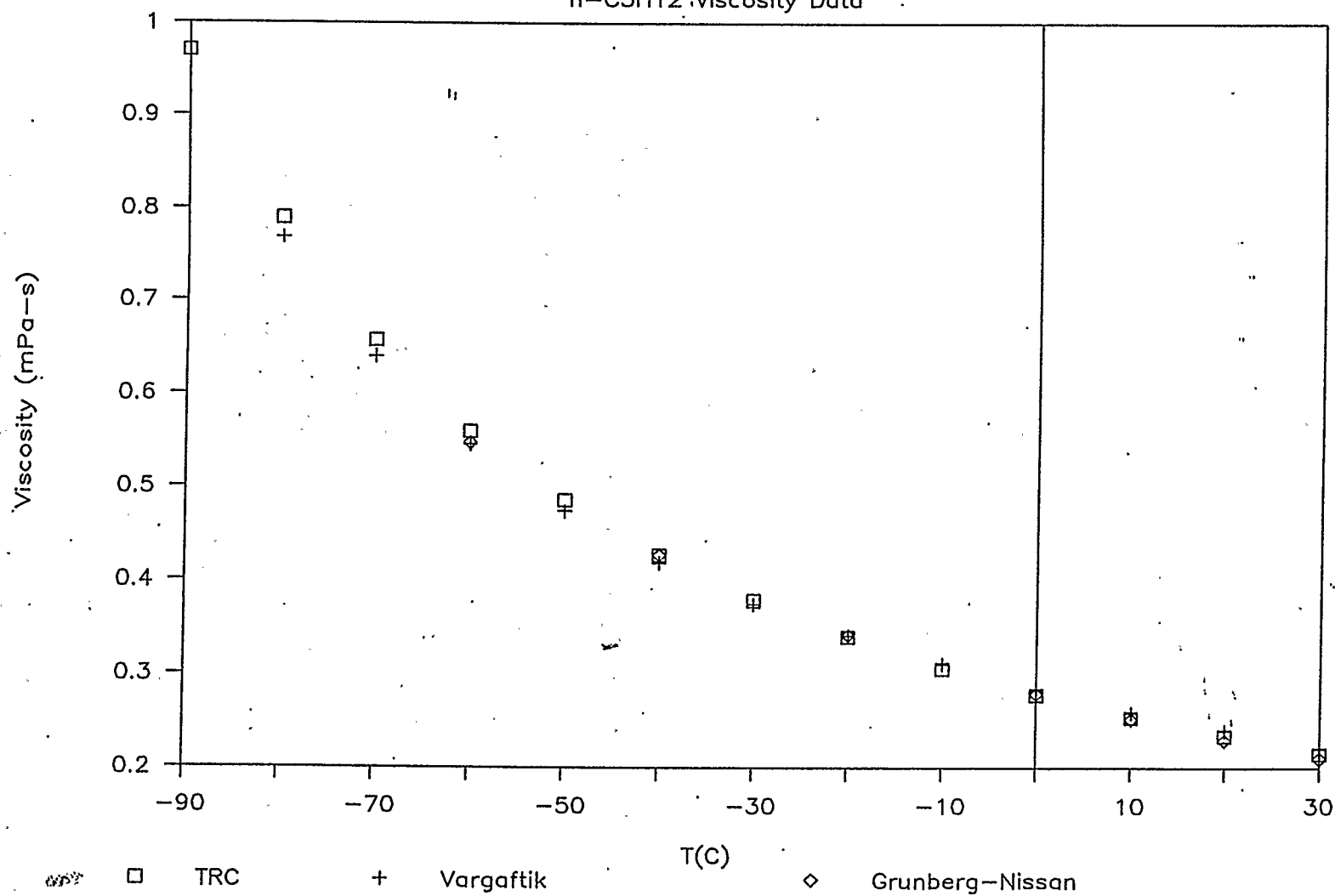
T(C)	Experimental Viscosity (mPa s)			
	1	2	3	Selected
-90	0.97			0.97
-80	0.789	0.768		0.789
-70	0.657	0.640		0.657
-60	0.560	0.546	0.548	0.560
-50	0.486	0.474		0.486
-40	0.427	0.419	0.427	0.427
-30	0.379	0.375		0.379
-20	0.340	0.341	0.342	0.340
-10	0.306	0.311		0.306
0	0.278	0.283	0.279	0.278
10	0.254	0.259	0.252	0.254
20	0.234	0.240	0.229	0.234
30*	0.215	0.220	0.210	0.215
40		0.191		0.191
50		0.177		0.177
60		0.162		0.162
70		0.149		0.149
80		0.136		0.136
90		0.125		0.125

* - Normal Boiling Point

Sources: 1 - TRC
2 - Vargaftik (Ely and Hanley)
3 - Grunberg & Nissan

Figure 1

n-C5H12 Viscosity Data



4.2 Component Properties

The molecular weight, normal boiling point, critical properties and accentric factor for all the compounds in the database were either taken from the database of Ely and Hanley's TRAPP program (Ely and Hanley, 1981) or from the database of Reid et al (1986). These properties are listed in Appendix B.

CHAPTER 5
MODIFICATIONS OF THE ELY-HANLEY EXTENDED CORRESPONDING
STATES VISCOSITY PREDICTION METHOD

Originally, the shape factors $\theta_{i,o}$ and $\phi_{i,o}$ were determined by equating the compressibility factors and fugacity coefficients of the complex fluid of interest and the reference fluid. These equations were solved for the reducing ratios $f_{i,o}$ and $h_{i,o}$ and from the definitions of these parameters, $\theta_{i,o}$ and $\phi_{i,o}$ were determined. Shape factors obtained in this manner provide reasonable estimates for liquid viscosities of similar compounds to the reference fluid. However, Hanley (1976) stated that shape factors obtained from thermodynamic data could not represent adequately, at high densities, fluids which did not correspond with the reference fluid. As stated in Chapter 3, this was corrected for by applying a correction factor based on modified Enskog theory, thus complicating the model.

An alternative approach is to modify the procedure for determining the shape factors. That is, instead of solving the conformal equations given in Chapter 3 for the shape factors, equations more convenient for viscosity could be solved. For this study, propane was chosen as the reference fluid and although a propane reference eliminates this problem for some compounds, the problem still persists for very dissimilar compounds, such as naphthenes and some aromatics (Ely, 1984).

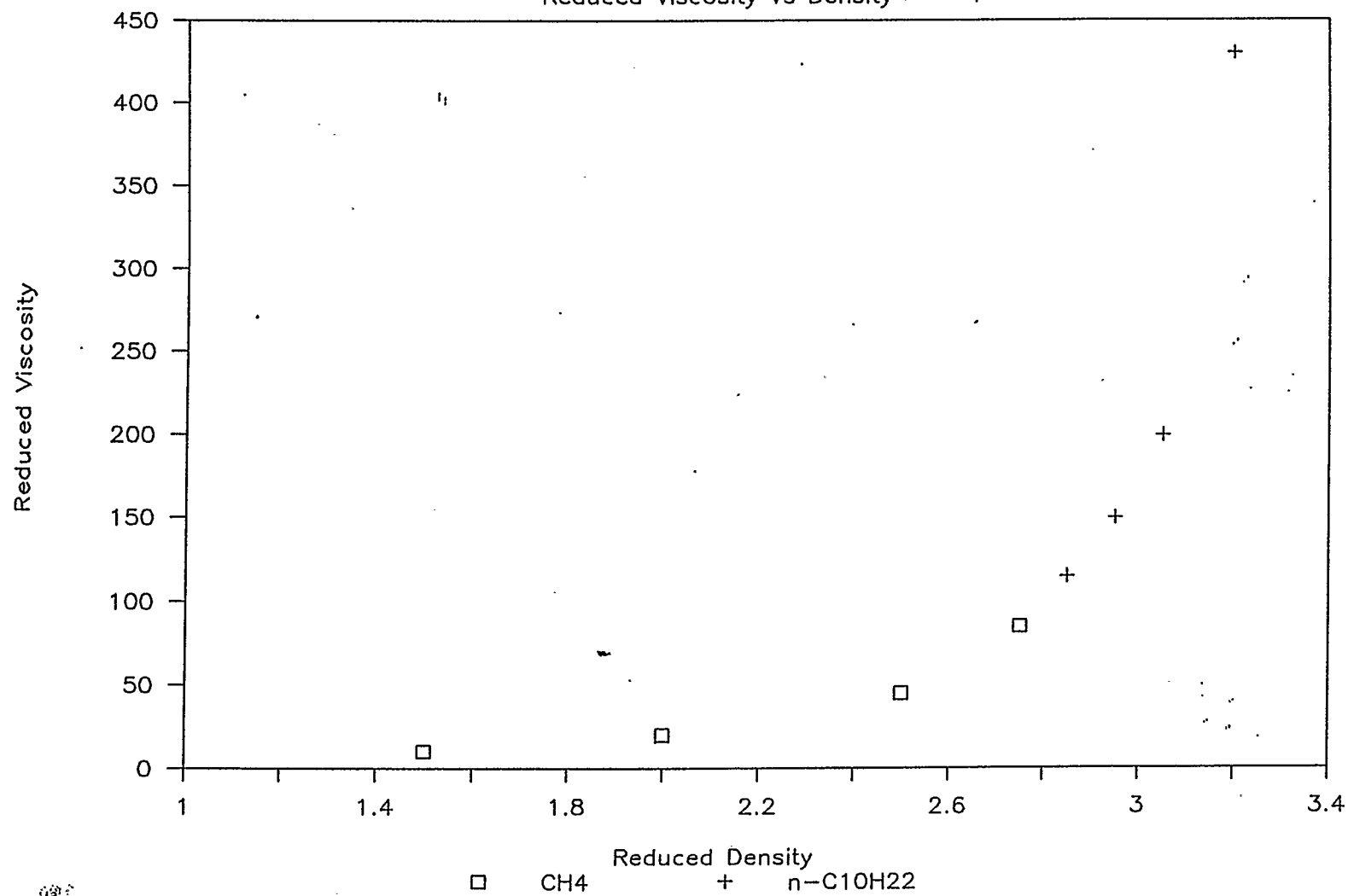
The major modification made to the existing method was in the determination of the shape factors. To provide values of the shape factors directly for viscosity, experimental viscosities were input into the existing model and corresponding values of $\theta_{i,o}$ were calculated while $\phi_{i,o}$ was set to equal to unity. This approach was necessary because the viscosity model only provided one equation in two unknowns, T_o and ρ_o and ultimately $\theta_{i,o}$ and $\phi_{i,o}$. Therefore, to reduce the model to a single unknown, one of the shape factors had to be set to a known value or eliminated. The shape factor $\phi_{i,o}$ was set equal to unity because its value usually does not deviate from unity as much as $\theta_{i,o}$ and because the viscosity calculation is significantly more sensitive to the value of $\theta_{i,o}$ than it is to $\phi_{i,o}$. This was demonstrated by observing the deviation in the shape factors and predicted viscosity when setting one of the shape factors equal to unity and calculating the other. The results, shown in Table 6, indicate that $\phi_{i,o}$ typically deviates from unity by 0.1% to 1.5% resulting in the predicted viscosity deviating by 0.1% to 4.5%. Conversely, $\theta_{i,o}$ typically deviates from unity by 2.5% to 9.5% resulting in the predicted viscosity deviating 9.8% to 77.5%. The greater sensitivity to an energy shape factor, as opposed to a size shape factor, is the result of the viscosity surface being sensitive to the value of the reduced density at high values (Ely and Hanley, 1981). This effect is shown in Figure 2. The reduced density is a function of the temperature and pressure but, for liquids, is much more sensitive to the value of temperature, and hence $\theta_{i,o}$. Sensitivity to an energy

Table 6
Deviations of Shape Factors and Predicted Viscosities

Compound	$\phi = 1$		$\theta = 1$	
	% $\Delta \phi$	% $\Delta \eta$	% $\Delta \theta$	% $\Delta \eta$
n-Hexane	0.96	2.32	4.54	29.64
n-Hexadecane	0.57	3.45	9.53	77.55
Cyclopentane	1.17	2.01	3.07	21.16
n-Propylcyclopentane	0.78	2.25	5.33	40.06
Cyclohexane	0.92	1.91	3.45	25.28
n-Propylcyclohexane	1.38	4.47	4.28	35.98
Benzene	0.99	1.72	3.47	25.84
n-Butylbenzene	1.51	4.78	6.13	50.75
Ethylene	0.09	0.13	2.46	9.84
1-Hexene	0.58	1.33	4.34	28.34

Figure 2

Reduced Viscosity vs Density



parameter is also in accordance with the fact that liquid viscosity is predominantly a function of interacting force fields. This sensitivity to an energy term is not surprising since this also occurs in thermodynamics, as evidenced by binary interaction corrections applied to the pseudo critical temperature or energy parameters in an equation of state (Prausnitz and Gunn, 1958).

If the density of the fluid of interest is known, an alternative to setting $\phi_{i,o}$ equal to unity is to calculate $h_{i,o}$ directly from the relationship given by Equation 3.27. This effectively eliminates the shape factor $\phi_{i,o}$ from the calculation. However, in this case, the calculation of θ involves another level of iteration since P_o must initially be guessed to calculate the equivalent density of the reference fluid.

Since the viscosity model is non-linear in $\theta_{i,o}$, the secant method was used for solving the equation. Values of $\theta_{i,o}$ were generated by a computer program. An algorithm for the program is given in Table 7.

Although final values of $\theta_{i,o}$ were calculated with $\phi_{i,o}$ set equal to unity, it should be noted that some $\theta_{i,o}$ values were also calculated by the alternative procedure of eliminating $\phi_{i,o}$. When the corresponding values of $\theta_{i,o}$ calculated by the two methods were compared, they agreed very closely, only deviating from each other by 0.2% to 0.4%. Therefore, we concluded that it makes little difference which method is used to simplify the model to a single unknown.

The other modification made to the existing method was the calculation procedure for the reference fluid equivalent density.

Table 7

Algorithm for Calculating θ

Required Input: T_c, V_c, M

T, P, η_{exp}

Known Constants: $T_{c_o}, P_{c_o}, V_{c_o}, M_o$

$A_{v_p_o}, B_{v_p_o}, C_{v_p_o}, D_{v_p_o}$

$V_o^*, \omega_{\text{SRK}o}$

- (1) Guess θ_1
- (2) Calculate $h_1 = V_c/V_{c_o}, f_1 = \theta_1 T_c/T_{c_o}$
 $To_1 = T/f_1, Tro_1 = To_1/T_{c_o}, Po_1 = P_{h_1}/f_1$
- (3) Calculate $P_{\text{vapo}_1} = f(To_1, T_{c_o}, P_{c_o}, A_{v_p_o}, B_{v_p_o}, C_{v_p_o}, D_{v_p_o})$
- (4) Calculate $\rho_{o1} = f(To_1, Po_1)$
 if $Tro_1 < 0.95$ then use $\text{COSTALD}(Tro_1, Po_1, P_{c_o}, P_{\text{vapo}_1}, V_o^*, \omega_{\text{SRK}o})$
 if $Tro_1 > 0.95$ then use 32 term BWR Equation of State
- (5) Calculate $\eta_{o1} = f(To_1, \rho_{o1})$
- (6) Calculate $\eta_1 = \eta_{o1}(To_1, \rho_{o1}) (M/M_o)^{1/2} f_1^{1/2} h_1^{-2/3}$
- (7) Guess $\theta_2, \theta = \theta_2$
- (8) Calculate $h_2 = V_c/V_{c_o}, f_2 = \theta_2 T_c/T_{c_o}$
 $To_2 = T/f_2, Tro_2 = To_2/T_{c_o}, Po_2 = P_{h_2}/f_2$
- (9) Calculate $P_{\text{vapo}_2} = f(To_2, T_{c_o}, P_{c_o}, A_{v_p_o}, B_{v_p_o}, C_{v_p_o}, D_{v_p_o})$
- (10) Calculate $\rho_{o2} = f(To_2, Po_2)$
 if $Tro_2 < 0.95$ then use $\text{COSTALD}(Tro_2, Po_2, P_{c_o}, P_{\text{vapo}_2}, V_o^*, \omega_{\text{SRK}o})$

Table 7 (continued)

Algorithm for Calculating θ

if $Tro_2 > 0.95$ then use 32 term BWR Equation of State

(11) Calculate $\eta_{o2} = f(To_2, \rho_{o2})$

(12) Calculate $\eta_2 = \eta_{o2}(To_2, \rho_{o2}) (M/Mo)^{1/2} f_2^{1/2} h_2^{-2/3}$

(13) $\theta_2 = \theta$

$$\theta = \theta_2 - (\eta_2 - \eta_{exp})(\theta_2 - \theta_1)/(\eta_2 - \eta_1)$$

$$\theta_1 = \theta_2$$

$$\eta_1 = \eta_2$$

Calculate $h = Vc/Vc_o$, $f = \theta Tc/Tc_o$

$$To = T/f, \quad Tro = To/Tc_o, \quad Po = Ph/f$$

Calculate $Pvapo = f(To, Tc_o, Pc_o, Avp_o, Bvp_o, Cvp_o, Dvp_o)$

Calculate $\rho_o = f(To, Po)$

if $Tro < 0.95$ then use $COSTALD(Tro, Po, Pc_o, Pvapo, V_o^*, \omega_{SRKo})$

if $Tro > 0.95$ then use 32 term BWR Equation of State

Calculate $\eta_o = f(To, \rho_o)$

Calculate $\eta = \eta_o(To, \rho_o) (M/Mo)^{1/2} f^{1/2} h^{-2/3}$

$$\eta_2 = \eta$$

(14) if $\theta - \theta_2 > 1E-6$ go to 13

(15) converged, output θ

Since the predicted liquid viscosity calculation is sensitive to the value of this density, an accurate calculation method is required. The 32 term BWR type complex equation of state, given in Table 1, is used in the existing TRAPP method. However, difficulties were encountered in the iterative solution of the equation, especially for compounds with molecular weights greater than 400 g/gmol (Johnson et al, 1987, Pedersen et al, 1984). Specifically, the equation of state converged to an incorrect root or did not converge at all. To avoid such difficulties, the corresponding states liquid density method, COSTALD (Hankinson and Thomson, 1979, Thomson, Brobst and Hankinson, 1982), has been substituted to calculate the reference fluid equivalent density. This non-iterative method, shown in Table 8, is much simpler and faster than the existing complex equation of state. The average deviation in the calculation of the reference fluid equivalent density for the COSTALD method is 0.295% compared to 0.25% for the existing method, an insignificant sacrifice in accuracy. It should be noted here that cubic equations of state were briefly considered but were rejected because none could not provide liquid densities consistently within 1% of experimental values.

Table 8
COSTALD Density Calculation Method*

$$V_s = V^* V_r^{(0)} [1 - \omega_{SRK} V_r^{(\delta)}]$$

$$V_r^{(0)} = 1 + a(1 - Tr)^{1/3} + b(1 - Tr)^{2/3} + c(1 - Tr) + d(1 - Tr)^{4/3}$$

$$V_r^{(\delta)} = (e + fTr + gTr^2 + hTr^3) / (Tr - 1.00001)$$

$$V = V_s \left(1 - C \ln \frac{B + P}{B + P_v} \right)$$

$$B = Pc [-1 + a(1 - Tr)^{1/3} + b(1 - Tr)^{2/3} + d(1 - Tr) + e(1 - Tr)^{4/3}]$$

$$e = \exp(f + g\omega_{SRK} + h\omega_{SRK}^2)$$

$$C = j + k\omega_{SRK}$$

* numerical values of constants are given in Appendix C,
Hankinson and Thomson (1979) and Thomson et al (1982)

CHAPTER 6

RESULTS AND DISCUSSION

6.1 Shape Factor Correlations

For each component in the database, θ was calculated over the entire temperature range of the data. For most compounds, this range was from approximately the freezing temperature to a reduced temperature of 0.7 to 0.9. The data for each component are summarized in Appendix A.

Based on the findings of Ely (1984), θ was assumed to only be a function of temperature. For each component in the database, θ was plotted against reduced temperature and Figures 3 and 4 show typical plots for n-hexadecane and benzene. In Figures 3 and 4, it can be seen that θ is a slightly curved negative sloping function of reduced temperature. However, for some compounds, θ showed an irregular trend, as shown in Figure 5 for n-hexane. This can be attributed to three possibilities:

- (i) ϕ being set equal to unity.
- (ii) deviations in the calculation of the reference fluid equivalent density.
- (iii) uncertainty in the experimental viscosity data.

The first possibility was eliminated because even if the density of the compound of interest was known and the alternate method of eliminating ϕ was used to calculate θ , the trend persisted. The second possibility

Figure 3

n-C16H34 Theta vs Tr

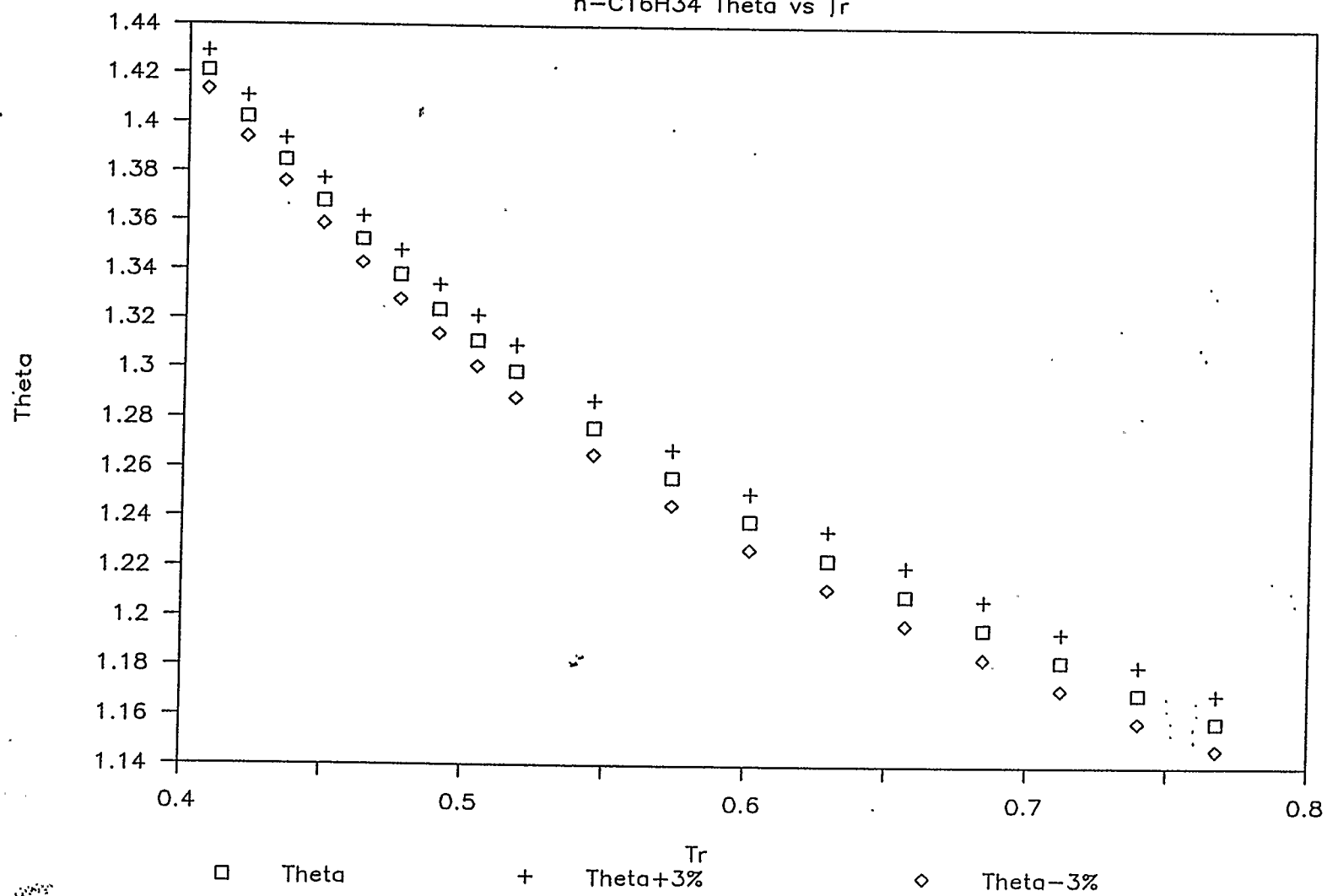


Figure 4

Benzene Theta vs Tr

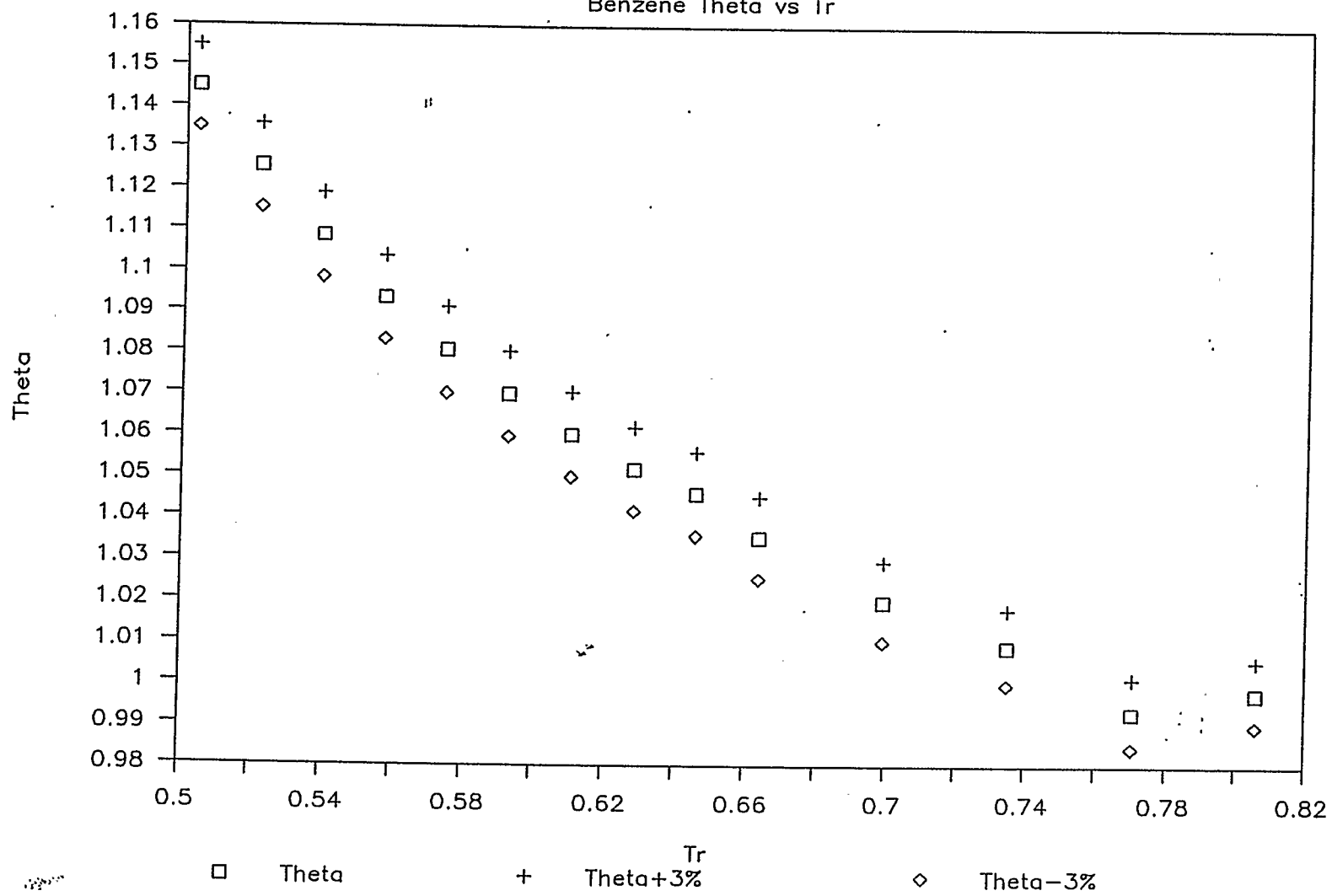
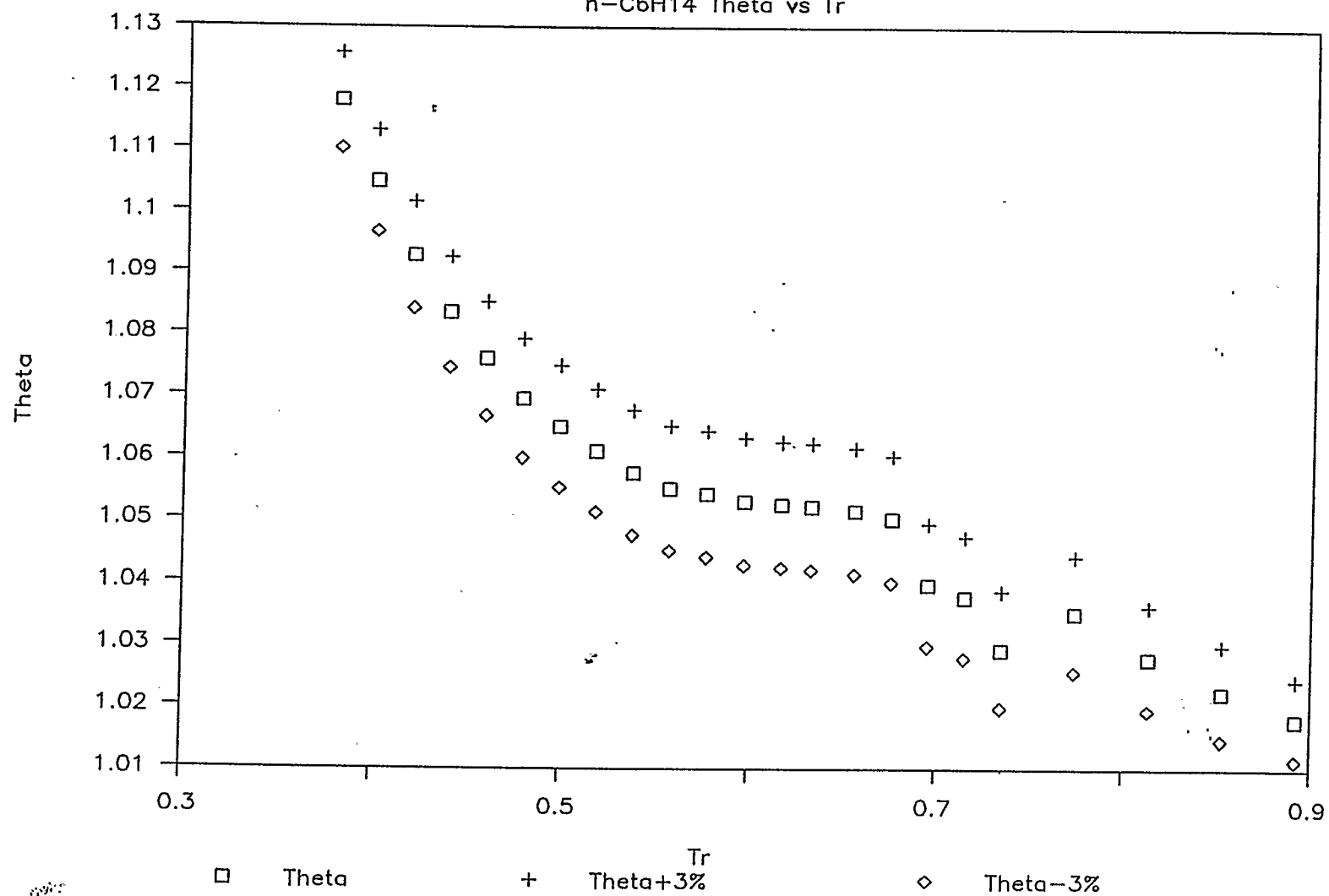


Figure 5

n-C6H14 Theta vs Tr



was eliminated because applying a correction to the calculation of the reference fluid equivalent density made no difference to the trend. Therefore, the irregular trends of θ for some compounds were attributed to uncertainty in the experimental viscosity data. To overcome this difficulty, θ was calculated at $\pm 3\%$ of each viscosity point and error bars were plotted. The regular trend of θ was then fit within this error band. In general, shape factors had to be within 0.5% to 1.0% to yield a predicted viscosity within 3%.

The variation of θ with reduced temperature could be modelled by several different functions. Initially, it appeared that this variation was similar to that of viscosity as a function of temperature. Two empirical functions for the variation of viscosity with temperature are the Andrade equation (Reid et al, 1986) and the ASTM correlation (API, 1987), given below as Equations 6.1 and 6.2, respectively.

$$\ln \eta = A + B/T \quad (6.1)$$

$$\ln \ln(\eta + C) = A + B \ln T \quad (6.2)$$

As a first attempt, the variation of θ with reduced temperature was modelled with Equation 6.1. The function modelled the data reasonably well with the values of the constants regressed by the method of least squares. However, in order to apply this research to hydrocarbons not in the database and, in the future, to pseudocomponents, it is necessary to generalize the constants in the shape factor correlation

as functions of characterization parameters such as molecular weight, normal boiling point, critical properties or acentric factor. Plots of the regressed values of the constants as functions of characterization parameters showed the constants to be significantly scattered, without any trends for all the database components. Consequently, attempts at generalizing these constants were unsuccessful.

While empirically modelling the viscosity of bitumens, Mehrotra and Svrcek (1988) found that the constants of an Andrade-type equation varied significantly. Conversely, they found that the constant B of the ASTM-type viscosity correlation fell within a narrow range of values for the bitumens. Therefore as a second attempt, the variation of θ with reduced temperature was modelled with Equation 6.2. This function also modelled the data well but the regressed constants for the database components were still scattered from each other and showed no trends (Monnery et al, 1988).

It was realized at this point that any errors in the predicted values of the constants would propagate exponentially for these equations. Hence, it was decided to try a function similar to the existing simplified shape factor correlations. A second order term was added to account for the slight curvature. The resulting form of the variation of θ with reduced temperature is given below as Equation 6.3.

$$f = A + Bx + Cx^2 \quad (6.3)$$

$$\text{where } f = \frac{\theta T_c}{T_{c0}} \quad (6.4)$$

$$x = \ln Tr \quad (6.5)$$

The reducing ratio f was modelled instead of θ directly since it appeared to vary more uniformly. The regressed constants for the database components, shown in Table 9, were still scattered from each other for this correlation, although somewhat less than the previously attempted correlations. Generalization of these constants again proved very difficult. However, it was decided to observe the behavior of θ for one hydrocarbon family at a time.

Plotting θ versus reduced temperature for all the paraffin series revealed similar behavior for the paraffins with a molecular weight greater than 100 g/mol and to ensure uniformity, the curves were slightly extrapolated. The constants were then regressed again for C_8 , C_{10} , C_{12} , C_{14} , C_{17} and C_{19} . New values of the constants were modelled as a function of normal boiling point, T_b . This parameter was chosen because it is energy related, is mostly known and varies uniformly from component to component within a family. It was non-dimensionalized by dividing by T_{bo} , the normal boiling point of the reference fluid. It should be noted here, that the acentric factor was not used because its variation is not as uniform as that of T_b .

Generalization of the paraffins with a molecular weight less than 100 g/mol and of the other hydrocarbon families was performed in a similar manner. It was observed from the magnitude of θ and its variation with temperature that the cyclopentanes and cyclohexanes should be modelled as distinct groups, as opposed to all naphthenic compounds being modelled as one family. It was also observed for

Table 9
Regressed Constants for Shape Factor Correlation

Compound	A	B	C
Methane	1.03401	-0.14334	0.02468
Ethane	1.00853	-0.09122	0.00109
Propane	0.99280	-0.01229	0.00360
n-Butane	1.01631	-0.00585	0.01135
i-Butane	1.06522	-0.05060	0.02758
n-Pentane	0.99882	-0.03385	0.01989
i-Pentane	0.97741	-0.06373	0.10504
n-Hexane	1.01115	-0.05364	0.04642
n-Heptane	1.01291	-0.10171	0.06192
n-Octane	1.00994	-0.15881	0.04703
n-Nonane	1.05957	-0.03085	0.19390
n-Decane	1.06039	-0.07460	0.18982
n-Undecane	1.06341	-0.09819	0.20157
n-Dodecane	1.04940	-0.19711	0.12962
n-Tridecane	1.06374	-0.17039	0.17993
n-Tetradecane	1.06091	-0.22022	0.14589
n-Pentadecane	1.06741	-0.24124	0.13847
n-Hexadecane	1.07299	-0.25911	0.12815
n-Heptadecane	1.07788	-0.27291	0.12492
n-Octadecane	1.08213	-0.27268	0.12462
n-Nonadecane	1.11394	-0.21054	0.19327
n-Eicosane	1.14525	-0.15360	0.23206
Ethene	0.90595	-0.01528	0.02248
Propene	0.89381	-0.00809	0.08102
1-Butene	0.94361	-0.03868	0.05662
1-Pentene	0.94020	-0.03911	0.05662
1-Hexene	0.96007	-0.02986	0.07503
Cyclopentane	1.02180	-0.14699	0.03959
Methylcyclopentane	1.01704	-0.15547	0.06836
Ethylcyclopentane	1.01858	-0.09947	0.05731
n-Propylcyclopentane	1.04815	-0.13795	0.15413
Cyclohexane	1.06069	-0.05543	0.52580
Methylcyclohexane	0.96111	-0.29217	0.06924
Ethylcyclohexane	1.06642	-0.01473	0.19595
n-Propylcyclohexane	1.02729	-0.03036	0.19843
n-Butylcyclohexane	0.84795	-0.40072	0.03981
Benzene	0.93161	-0.20607	0.11234
Toluene	0.92187	-0.14014	0.06471
Ethylbenzene	0.96959	-0.03630	0.12486
o-Xylene	0.96848	-0.04682	0.15207
m-Xylene	0.96841	-0.02077	0.09417
p-Xylene	0.97120	-0.01597	0.12464
n-Propylbenzene	0.97526	-0.05369	0.16390
Isopropylbenzene	0.89841	-0.11985	0.11420
n-Butylbenzene	0.98476	-0.05064	0.17889
Naphthalene	0.98680	-0.01625	0.23084

naphthenes and aromatics that θ values for the base compounds (cyclopentane, cyclohexane and benzene) behaved somewhat differently from the rest of the compounds in each respective family.

For each family or group, the constants A, B and C were modelled as a linear or quadratic function of T_b/T_{bo} . The resulting functions are given in Table 10.

6.2 Predicted Viscosities

With the generalized and regressed values of the constants in the shape factor correlation, the viscosities predicted by the modified method were compared to experimental values. The results are summarized in Table 11. Also provided for comparison are the deviations from experimental values, of viscosities predicted by Ely and Hanley's TRAPP program (Ely and Hanley, 1981b) with the methane reference. The deviations of the TRAPP method were calculated from the same data points as the modified method. Only the average absolute deviations are shown because the maximum error is not a good measure of a method's reliability, since it often reflects the uncertainty or scatter of the experimental data.

The results show that the modified method, with the generalized shape factor constants (GMECS), consistently predicts liquid viscosities to within 6% to 8% of the experimental data for forty two of the forty six compounds tested. The viscosities of three other compounds (methylcyclohexane, ethylcyclohexane and m-xylene) are predicted within 10% . The only compound that is not predicted within

Table 10
Generalized Shape Factor Functions

Paraffins $M > 100$

$$A = 0.26272 + 0.75213 (T_b/T_{bo})$$

$$B = 0.45977 - 0.39881 (T_b/T_{bo})$$

$$C = -1.25725 + 1.18289 (T_b/T_{bo}) - 0.23304 (T_b/T_{bo})^2$$

Paraffins $M < 100$

$$A = 0.13215 + 0.85844 (T_b/T_{bo})$$

$$B = -0.27418 + 0.55865 (T_b/T_{bo}) - 0.29932 (T_b/T_{bo})^2$$

$$C = 0.04500 - 0.08811 (T_b/T_{bo}) + 0.04298 (T_b/T_{bo})^2$$

Olefins

$$A = 0.11160 + 0.79508 (T_b/T_{bo})$$

$$B = 0.0649 - 0.1001 (T_b/T_{bo}) - 0.0405 (T_b/T_{bo})^2$$

$$C = -0.0002 - 0.0010 (T_b/T_{bo}) + 0.0065 (T_b/T_{bo})^2$$

Cyclopentanes

$$A = 0.99771 + 0.13439 (T_b/T_{bo}) + 0.11630 (T_b/T_{bo})^2$$

$$B = -1.25286 + 1.40528 (T_b/T_{bo}) - 0.49602 (T_b/T_{bo})^2$$

$$C = 0.28865 - 0.40786 (T_b/T_{bo}) + 0.14870 (T_b/T_{bo})^2$$

Table 10 (continued)
Generalized Shape Factor Functions

Cyclohexanes

$$A = 0.27932 + 0.67150 (T_b/T_{bo}) + 0.03507 (T_b/T_{bo})^2$$

$$B = -11.1327 + 11.4363 (T_b/T_{bo}) - 3.0526 (T_b/T_{bo})^2$$

$$C = 7.3664 - 8.4663 (T_b/T_{bo}) + 2.4357 (T_b/T_{bo})^2$$

Aromatics

$$A = 0.88181 + 0.23520 (T_b/T_{bo}) + 0.07400 (T_b/T_{bo})^2$$

$$B = -7.6852 + 8.8326 (T_b/T_{bo}) - 2.5330 (T_b/T_{bo})^2$$

$$C = 1.18301 - 1.36990 (T_b/T_{bo}) + 0.39911 (T_b/T_{bo})^2$$

Table 11
Predicted Viscosity Results
Average Absolute Deviation(%)

Compound	RMECS	GMECS	TRAPP
Methane	2.73	2.94	1.49
Ethane	2.15	3.30	6.83
Propane	1.05	1.20	4.73
n-Butane	0.77	4.57	3.82
i-Butane	1.17	24.27	25.59
n-Pentane	1.61	3.05	4.04
i-Pentane	0.91	6.25	9.22
n-Hexane	2.47	3.74	5.03
n-Heptane	2.93	4.28	4.05
n-Octane	1.77	2.14	3.88
n-Nonane	1.47	2.22	2.54
n-Decane	1.07	1.46	1.57
n-Undecane	1.01	1.75	1.63
n-Dodecane	1.29	1.67	1.62
n-Tridecane	1.13	2.17	1.93
n-Tetradecane	1.03	2.01	1.46
n-Pentadecane	1.21	2.38	2.86
n-Hexadecane	1.13	2.15	4.15
n-Heptadecane	1.01	2.19	3.65
n-Octadecane	1.23	2.29	3.80
n-Nonadecane	0.67	3.37	4.02
n-Eicosane	0.33	3.71	15.41
Ethene	0.80	2.76	1.27
Propene	1.48	5.23	5.64
1-Butene	0.91	1.58	12.49
1-Pentene	1.24	1.76	42.58
1-Hexene	1.42	1.53	19.24
Cyclopentane	0.05	2.84	29.67
Methylcyclopentane	0.51	3.88	27.81
Ethylcyclopentane	0.52	1.72	12.75
n-Propylcyclopentane	1.98	2.17	5.32
Cyclohexane	1.09	4.93	54.34
Methylcyclohexane	0.39	9.60	34.53
Ethylcyclohexane	0.94	8.10	31.33
n-Propylcyclohexane	1.15	2.26	34.03
n-Butylcyclohexane	1.57	1.73	7.30
Benzene	1.53	2.33	10.98
Toluene	2.97	4.38	5.02
Ethylbenzene	1.20	1.64	9.08
o-Xylene	0.87	6.11	5.47
m-Xylene	0.89	9.34	23.10
p-Xylene	0.30	5.73	17.70
n-Propylbenzene	1.18	4.92	9.27
Isopropylbenzene	0.30	1.37	4.27
n-Butylbenzene	1.08	4.25	13.66
Naphthalene	0.71	5.68	12.30

the uncertainty of the data, is isobutane which deviates by 24.3% . Typically, hydrocarbon isomers have different values of physical constants and calculated properties at the same conditions than either the corresponding normal compound or other isomers (Reid et al, 1986). This is due to the different chemical structure of the isomers. Consequently, predicting trends of physical constants or properties for normal compounds seldom results in these trends providing accurate values for isomers of the normal compounds. Accordingly, the deviation in predicted viscosity for isobutane is due to the fact that it has a lower normal boiling point than normal butane, resulting in lower values of the shape factor constants and hence lower values of the reducing ratio "f" at corresponding reduced temperatures. This ultimately results in lower predicted viscosities for isobutane when in fact the actual viscosities are greater than those of normal butane at corresponding reduced temperatures. The viscosities predicted by the modified method with the regressed constants (RMECS) are consistently predicted within 2% to 3% for all forty six compounds tested. At the same time these results are attained, the calculation of the reference fluid equivalent density is much simpler and faster than the existing method.

In comparison, the existing Ely and Hanley extended corresponding states method predicts reasonable liquid viscosities for paraffins, usually within about 5% error. However, the predicted liquid viscosities for naphthenic compounds are much worse, as well as inconsistent, with average errors ranging anywhere from about 5% to

55%. The predicted liquid viscosities of aromatic compounds are somewhat better than naphthenic compounds, with average errors ranging from about 5% to 20%. Results for olefins are similar to naphthenic compounds with errors ranging from about 1% to 43%.

The predicted and experimental viscosities for each compound over the entire temperature range of the data are shown in Appendix A. These data reflect the good agreement between the modified method and the experimental values, as shown in Table 11. It can be seen that, the maximum error of the modified method occurs at reduced temperatures less than 0.5. At these reduced temperatures, the predicted viscosity is slightly low for most compounds. For the xylenes, however, the predicted viscosities at these reduced temperatures is slightly high. The maximum error is typically in the order of 6% to 10% .

CHAPTER 7

CONCLUSIONS

The following conclusions were reached during this study of pure component liquid hydrocarbon viscosity prediction by the extended corresponding states method:

- (1) The key to predicting accurate viscosities is obtaining the the correct magnitude of the shape factors, the variation of these shape factors with temperature and the proper functional form to fit this variation. The existing method for determining the shape factors does not provide values which result in consistent and accurate predicted liquid viscosities for non-paraffinic compounds.
- (2) The method for determining the shape factors presented in this research provides better values of the factors resulting in improved liquid viscosity predictions, usually within about 6% of the experimental values.
- (3) The viscosity of some hydrocarbon isomers, such as isobutane, are not satisfactorily predicted by a generalized method based on characterization parameters.
- (4) The method is more sensitive to the value of the energy shape factor, θ , than it is to the size shape factor, ϕ .
- (5) The shape factor θ is a slightly curved, negatively sloping function of reduced temperature.
- (6) Magnitudes of the shape factor θ and the slope of θ with respect to

temperature vary from component to component. This variation occurs in a manner such that generalizing θ as a function of a characterization parameter within a hydrocarbon family is attainable, but a generalization for all components is very difficult. Furthermore, cyclic compounds which have different structures must be generalized as distinct groups, as evidenced by the cyclopentanes and cyclohexanes.

- (7) Substituting the COSTALD method for calculating the reference fluid equivalent density eliminates the problems caused by the complex equation of state, with an insignificant sacrifice in accuracy.
- (8) Reliable published data is limited, especially for temperatures above the normal boiling point.

CHAPTER 8

RECOMMENDATIONS FOR FUTURE WORK

- (1) Attempts should be made to decrease the range of the shape factor θ required for accurate viscosity prediction by reintroducing the shape factor ϕ into the method. To solve for the two unknowns, ρ_0 and T_0 , simultaneously solve two equations which equate:
 - 1) the viscosities of the fluid of interest and the reference fluid
 - and 2) the compressibility factors of the fluid of interest and the reference fluid.Use the Lee-Kesler equation of state to calculate the compressibility factors. For each component, redetermine the values of the shape factors and their variation with reduced temperature. Finally, generalize the shape factor correlations to predict the new shape factors.
- (2) The viscosities of isomers should be correlated as functions of characterization parameters and the corresponding normal component viscosities. Investigate applying an approach similar to that which Reidel (1963) developed for critical properties based on the Platt number.
- (3) The existing mixing rules should be evaluated by predicting the viscosities of binary and ternary mixtures. Investigate the possibility of including a binary interaction parameter in the mixing rules and determine what parameters it would be most sensitive to.
- (4) After completion of the previous recommendations, evaluate the

method for predicting the viscosities of light oils, knowing the complete composition. Then attempt heavier hydrocarbons which have been characterized.

- (5) If the method is still unsuccessful for heavy hydrocarbons, determine the values of the shape factors that are necessary to accurately predict the viscosities of the components which make up the complex mixture. Investigate the necessity of a heavier reference fluid for such compounds.
- (6) Obtain more experimental viscosity data not available in the literature. Either generate the data experimentally or try to obtain the data from sources such as the National Bureau of Standards in the United States, the DECHEMA viscosity database, the AIChE Dippr database or company files.

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APPENDICES

APPENDIX A

Experimental and Predicted Viscosities for Database Components

Table A-1
Methane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-170.00	0.5413	0.1420	0.1372	0.1377
101.325	-163.15	0.5772	0.1230	0.1196	0.1185
250.000	-153.15	0.6297	0.0975	0.0989	0.0968
400.000	-143.15	0.6822	0.0810	0.0823	0.0802
700.000	-133.15	0.7347	0.0673	0.0686	0.0670
1100.000	-123.15	0.7872	0.0557	0.0567	0.0561
1800.000	-113.15	0.8396	0.0465	0.0462	0.0472
2600.000	-103.15	0.8921	0.0376	0.0357	0.0385

Figure A-1

CH₄ Viscosity Data

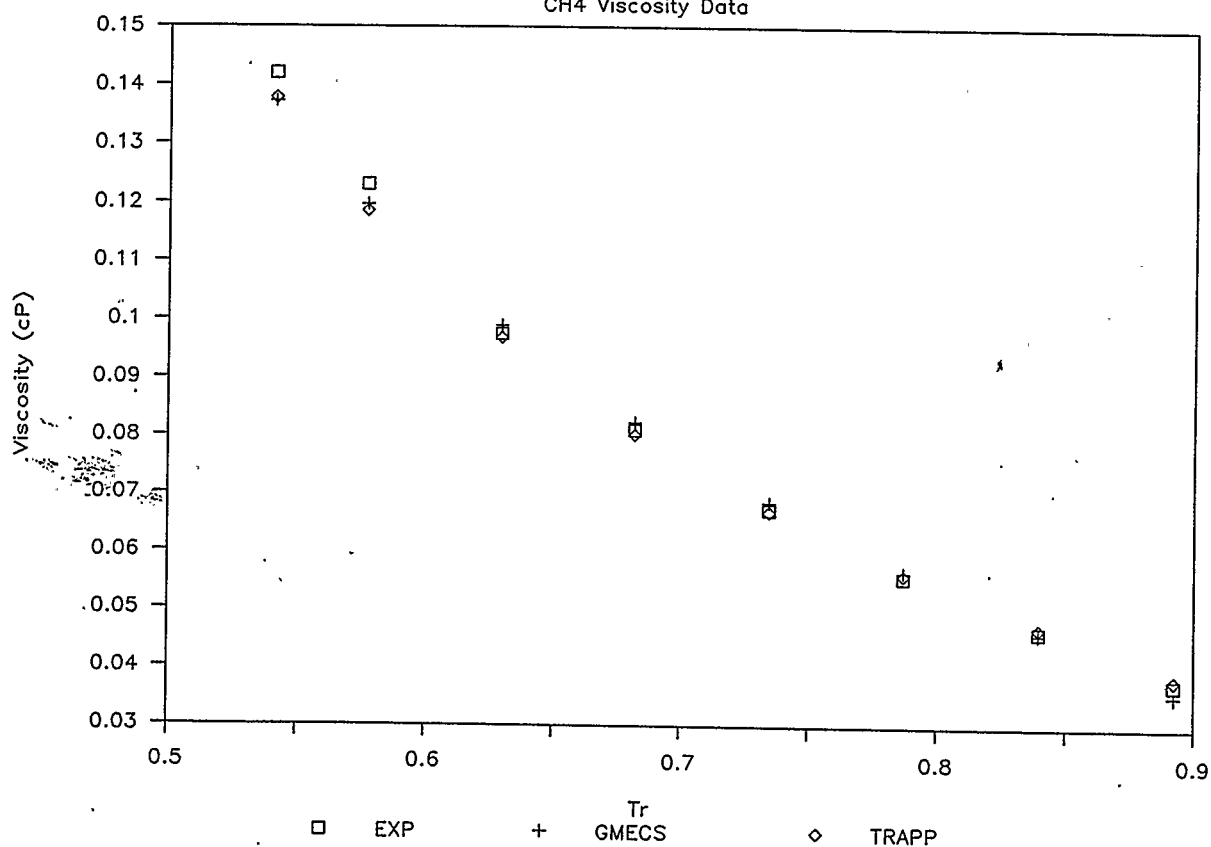


Table A-2
Ethane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-170.00	0.3378	0.8030	0.7444	
101.325	-160.00	0.3706	0.5720	0.5665	
101.325	-150.00	0.4033	0.4410	0.4496	0.5228
101.325	-140.00	0.4361	0.3580	0.3677	0.4119
101.325	-130.00	0.4688	0.3000	0.3076	0.3343
101.325	-120.00	0.5016	0.2560	0.2617	0.2775
101.325	-110.00	0.5343	0.2210	0.2255	0.2344
101.325	-100.00	0.5671	0.1940	0.1963	0.2007
101.325	-90.00	0.5998	0.1710	0.1721	
250.000	-80.00	0.6326	0.1470	0.1520	0.1518
500.000	-60.00	0.6981	0.1190	0.1198	0.1179
900.000	-40.00	0.7636	0.0959	0.0948	0.0928
1650.000	-20.00	0.8291	0.0755	0.0746	0.0733
2600.000	0.00	0.8946	0.0580	0.0567	0.0569

Figure A-2

C₂H₆ Viscosity Data

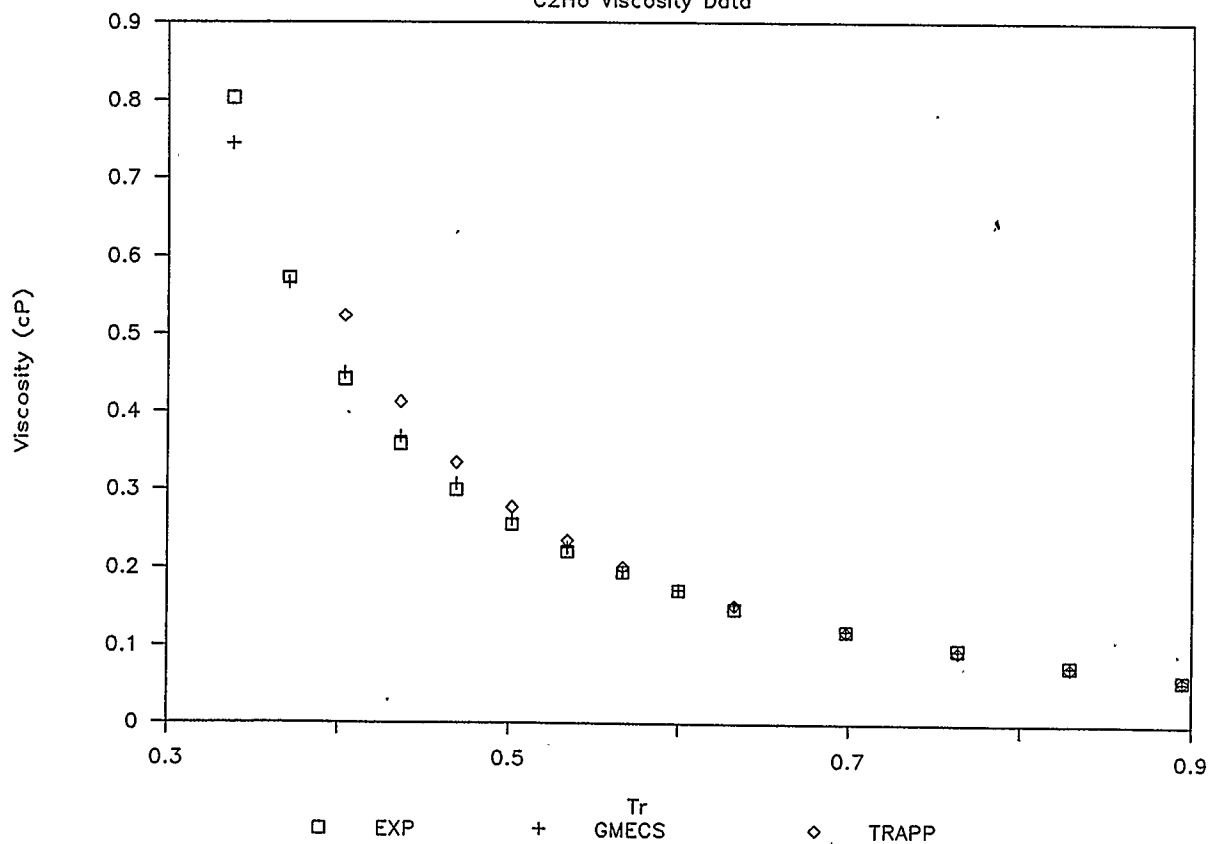


Table A-3
Propane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-173.15	0.2704	3.8190	3.6297	
101.325	-163.15	0.2974	2.2870	2.2121	
101.325	-153.15	0.3245	1.5260	1.4967	
101.325	-143.15	0.3515	1.0850	1.0883	
101.325	-133.15	0.3786	0.8320	0.8330	0.8390
101.325	-123.15	0.4056	0.6590	0.6620	0.6586
101.325	-113.15	0.4326	0.5460	0.5412	0.5324
101.325	-103.15	0.4597	0.4530	0.4522	0.4405
101.325	-93.15	0.4867	0.3820	0.3843	0.3713
101.325	-73.15	0.5408	0.2870	0.2881	0.2750
101.325	-53.15	0.5949	0.2240	0.2236	0.2122
250.000	-33.15	0.6490	0.1800	0.1777	0.1681
450.000	-13.15	0.7030	0.1440	0.1431	0.1356
600.000	-3.15	0.7301	0.1300	0.1288	0.1223
750.000	6.85	0.7571	0.1170	0.1159	0.1104
950.000	16.85	0.7842	0.1050	0.1043	0.0998
1200.000	26.85	0.8112	0.0959	0.0937	0.0903

Figure A-3

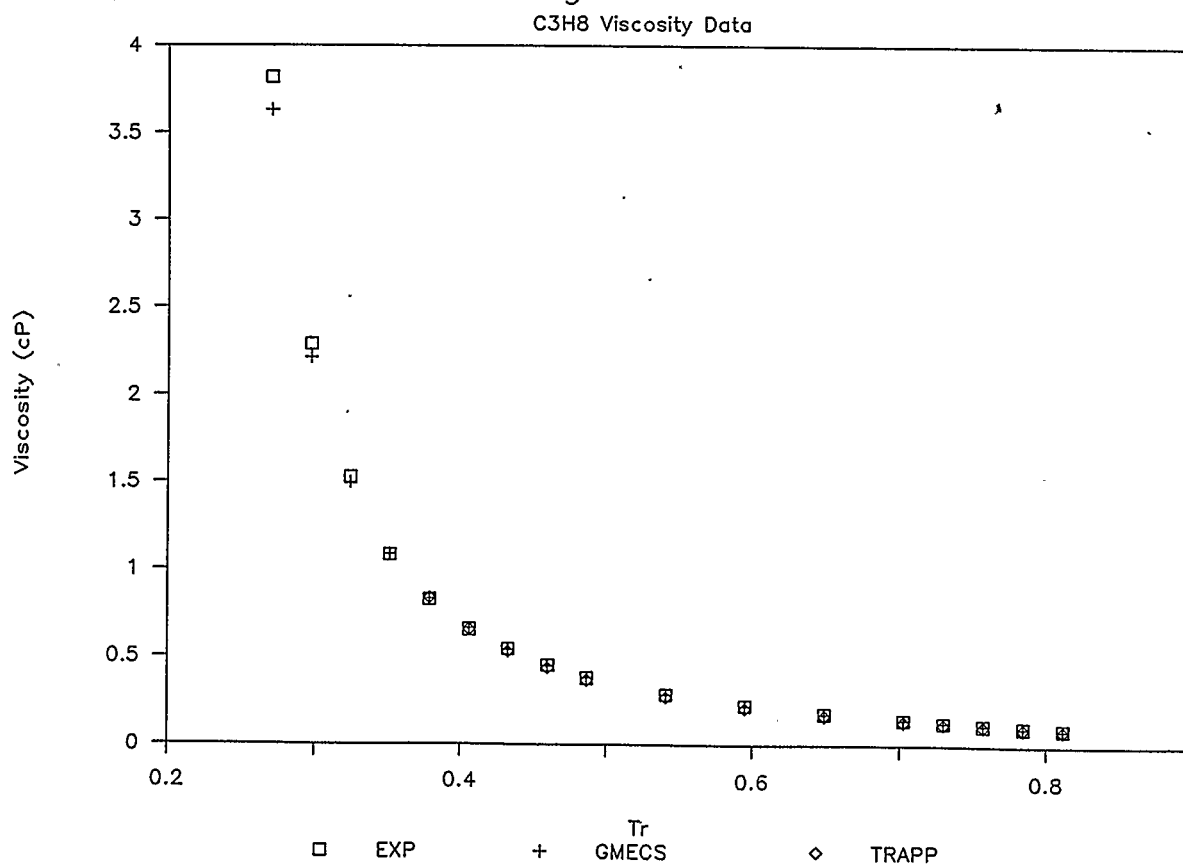


Table A-4
n-Butane Viscosity Data

P(kPa)	T(°C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-90.00	0.4308	0.6300	0.6059	
101.325	-80.00	0.4542	0.5340	0.5149	0.5410
101.325	-70.00	0.4778	0.4610	0.4437	0.4605
101.325	-60.00	0.5013	0.4020	0.3868	0.3972
101.325	-50.00	0.5249	0.3540	0.3404	0.3463
101.325	-40.00	0.5484	0.3140	0.3019	0.3047
101.325	-30.00	0.5719	0.2810	0.2695	0.2702
101.325	-20.00	0.5954	0.2520	0.2418	0.2411
101.325	-10.00	0.6189	0.2280	0.2178	0.2165
101.325	0.00	0.6425	0.2090	0.1970	0.1952
250.000	4.40	0.6528	0.2000	0.1890	0.1868
300.000	15.60	0.6792	0.1810	0.1697	0.1673
400.000	26.70	0.7053	0.1640	0.1529	0.1506

Figure A-4

N-C₄H₁₀ Viscosity Data

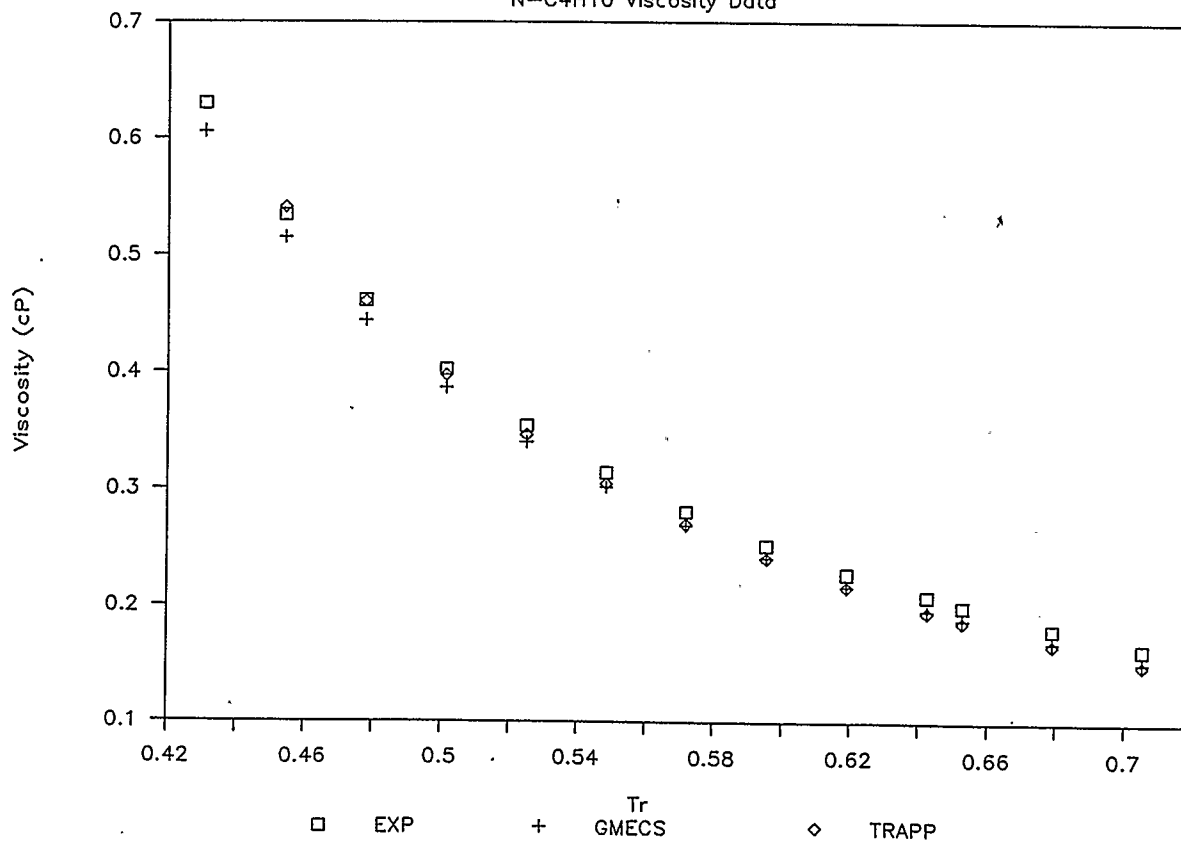


Table A-5
i-Butane Viscosity Data

P(kPa)	T(C)	Tr	- Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-80.00	0.4732	0.6260	0.4418	0.4496
101.325	-70.00	0.4977	0.5280	0.3825	0.3856
101.325	-60.00	0.5222	0.4520	0.3346	0.3347
101.325	-50.00	0.5467	0.3910	0.2953	0.2934
101.325	-40.00	0.5712	0.3420	0.2624	0.2593
101.325	-30.00	0.5957	0.3010	0.2345	0.2307
101.325	-20.00	0.6202	0.2670	0.2105	0.2065
101.325	-10.00	0.6447	0.2380	0.1897	0.1858

Figure A-5

I-C₄H₁₀ Viscosity Data

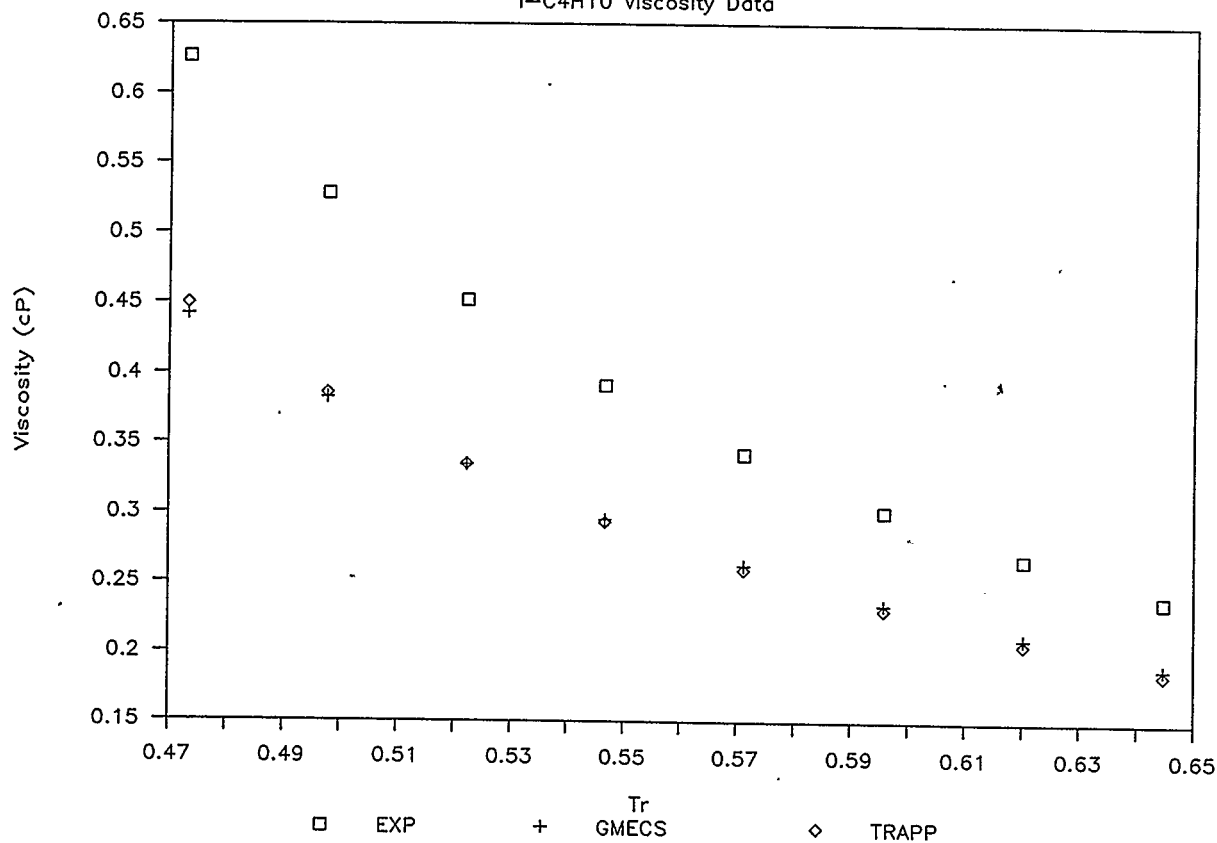


Table A-6
n-Pentane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-90.00	0.3899	0.9700	0.9884	
101.325	-80.00	0.4112	0.7890	0.8172	
101.325	-70.00	0.4325	0.6570	0.6889	0.7484
101.325	-60.00	0.4538	0.5600	0.5900	0.6315
101.325	-50.00	0.4750	0.4860	0.5119	0.5406
101.325	-40.00	0.4963	0.4270	0.4488	0.4684
101.325	-30.00	0.5176	0.3790	0.3970	0.4100
101.325	-20.00	0.5389	0.3400	0.3538	0.3620
101.325	-10.00	0.5602	0.3060	0.3172	0.3220
101.325	0.00	0.5815	0.2780	0.2860	0.2882
101.325	10.00	0.6028	0.2540	0.2589	0.2593
101.325	20.00	0.6241	0.2340	0.2353	0.2345
101.325	30.00	0.6453	0.2150	0.2144	0.2129
250.000	40.00	0.6666	0.1910	0.1964	0.1940
400.000	60.00	0.7092	0.1620	0.1652	0.1622
600.000	80.00	0.7518	0.1360	0.1397	0.1367
850.000	100.00	0.7944	0.1150	0.1182	0.1156
1200.000	120.00	0.8369	0.0963	0.0998	0.0977
1650.000	140.00	0.8795	0.0807	0.0836	0.0823

Figure A-6

N-C5H12 Viscosity Data

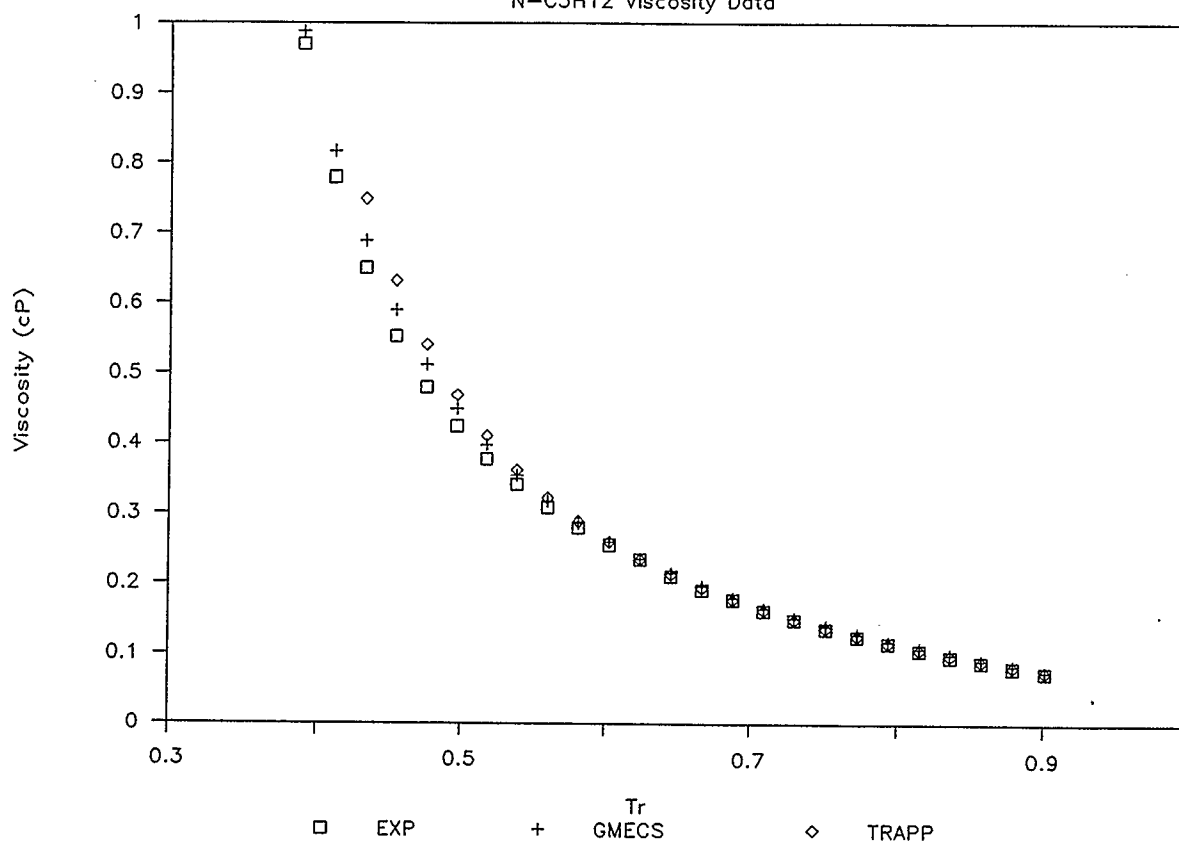


Table A-7
i-Pentane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-50.00	0.4847	0.5500	0.4719	0.4766
101.325	-40.00	0.5064	0.4700	0.4151	0.4153
101.325	-30.00	0.5281	0.4030	0.3681	0.3653
101.325	-20.00	0.5498	0.3520	0.3287	0.3239
101.325	-10.00	0.5715	0.3100	0.2952	0.2891
101.325	0.00	0.5932	0.2770	0.2664	0.2595
101.325	10.00	0.6150	0.2480	0.2414	0.2343
101.325	20.00	0.6367	0.2240	0.2195	0.2123
101.325	30.00	0.6584	0.2040	0.2001	0.1931

Figure A-7

I-C₅H₁₂ Viscosity Data

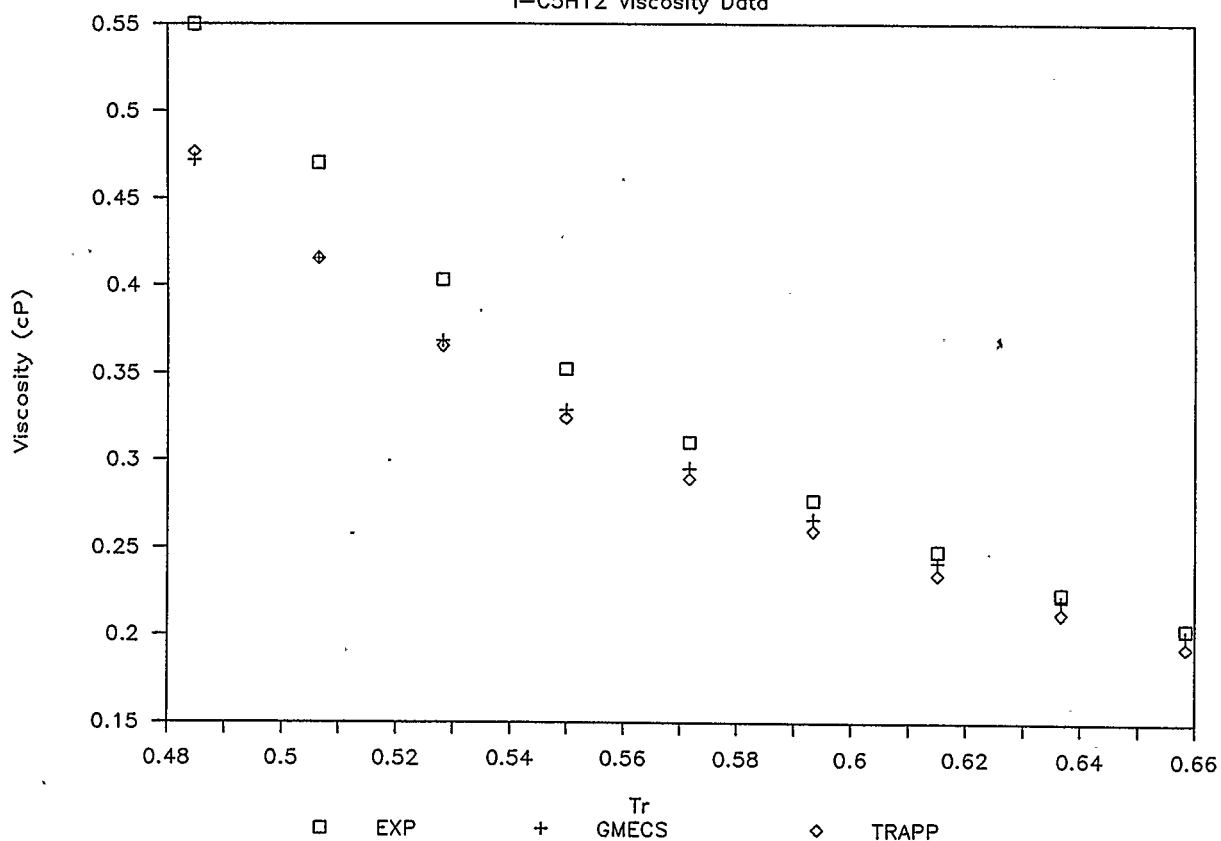


Table A-8
n-Hexane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-90.00	0.3606	1.8200	1.6102	
101.325	-80.00	0.3803	1.3800	1.2841	
101.325	-70.00	0.4000	1.0900	1.0513	
101.325	-60.00	0.4197	0.8850	0.8789	
101.325	-50.00	0.4394	0.7390	0.7475	0.8086
101.325	-40.00	0.4591	0.6300	0.6448	0.6883
101.325	-30.00	0.4787	0.5450	0.5626	0.5934
101.325	-20.00	0.4984	0.4790	0.4958	0.5171
101.325	-10.00	0.5181	0.4250	0.4405	0.4549
101.325	0.00	0.5378	0.3799	0.3941	0.4033
101.325	10.00	0.5575	0.3426	0.3547	0.3600
101.325	20.00	0.5772	0.3117	0.3209	0.3233
101.325	30.00	0.5969	0.2845	0.2915	0.2917
101.325	40.00	0.6166	0.2611	0.2658	0.2646
101.325	60.00	0.6559	0.2216	0.2229	0.2201
300.000	80.00	0.6953	0.1960	0.1893	0.1849
500.000	100.00	0.7347	0.1590	0.1616	0.1569
700.000	120.00	0.7741	0.1290	0.1384	0.1337
950.000	140.00	0.8135	0.1120	0.1186	0.1141

Figure A-8

N-C6H14 Viscosity Data

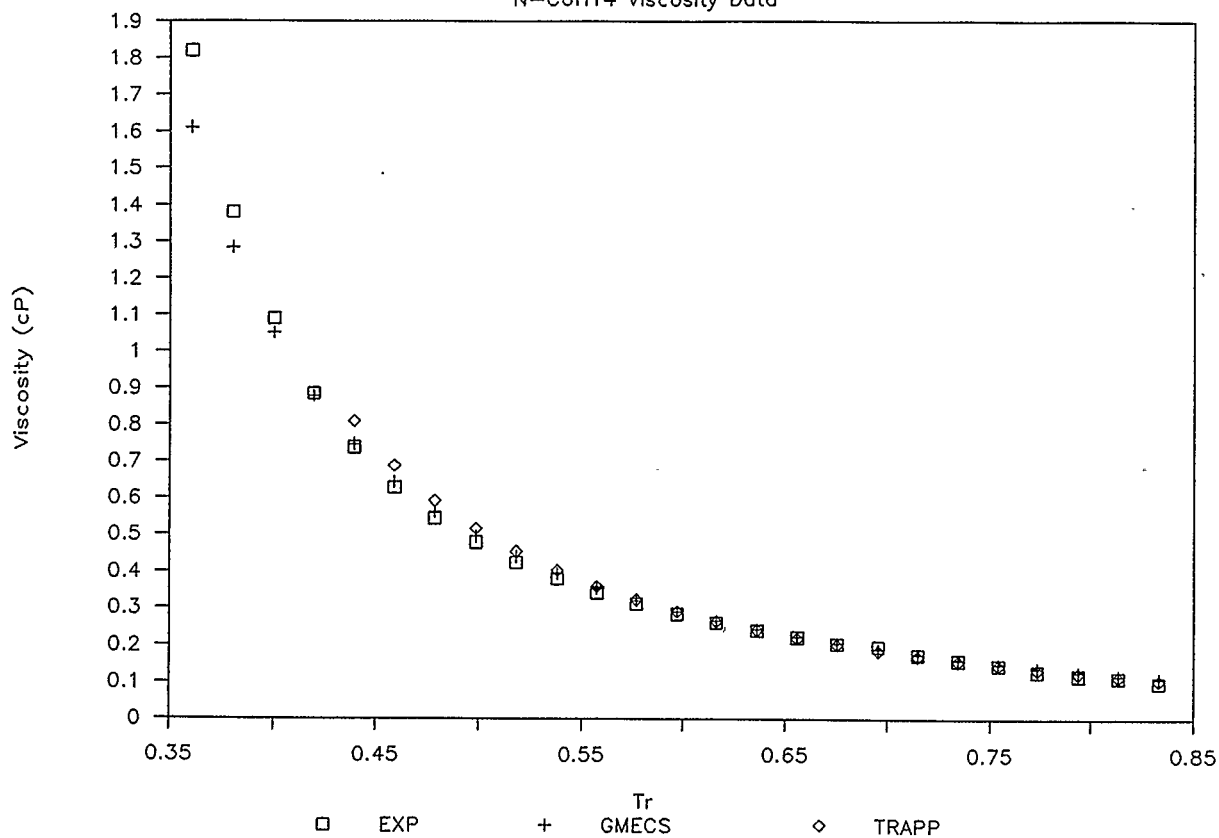


Table A-9
n-Heptane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-90.00	0.3391	3.7600	2.9251	
101.325	-80.00	0.3576	2.6000	2.1853	
101.325	-70.00	0.3761	1.9120	1.6969	
101.325	-60.00	0.3946	1.4720	1.3586	
101.325	-50.00	0.4131	1.1730	1.1148	
101.325	-40.00	0.4316	0.9624	0.9331	0.9989
101.325	-30.00	0.4502	0.8074	0.7940	0.8458
101.325	-20.00	0.4687	0.6896	0.6848	0.7257
101.325	-10.00	0.4872	0.5978	0.5974	0.6298
101.325	0.00	0.5057	0.5246	0.5261	0.5518
101.325	10.00	0.5242	0.4652	0.4671	0.4876
101.325	20.00	0.5427	0.4169	0.4176	0.4339
101.325	30.00	0.5612	0.3761	0.3755	0.3887
101.325	40.00	0.5798	0.3416	0.3394	0.3500
101.325	50.00	0.5983	0.3119	0.3081	0.3167
101.325	60.00	0.6168	0.2858	0.2807	0.2879
101.325	70.00	0.6353	0.2627	0.2566	0.2628
101.325	80.00	0.6538	0.2424	0.2351	0.2405
101.325	90.00	0.6723	0.2243	0.2160	0.2208
101.325	100.00	0.6908	0.2080	0.1987	0.2031

Figure A-9

N-C7H16 Viscosity Data

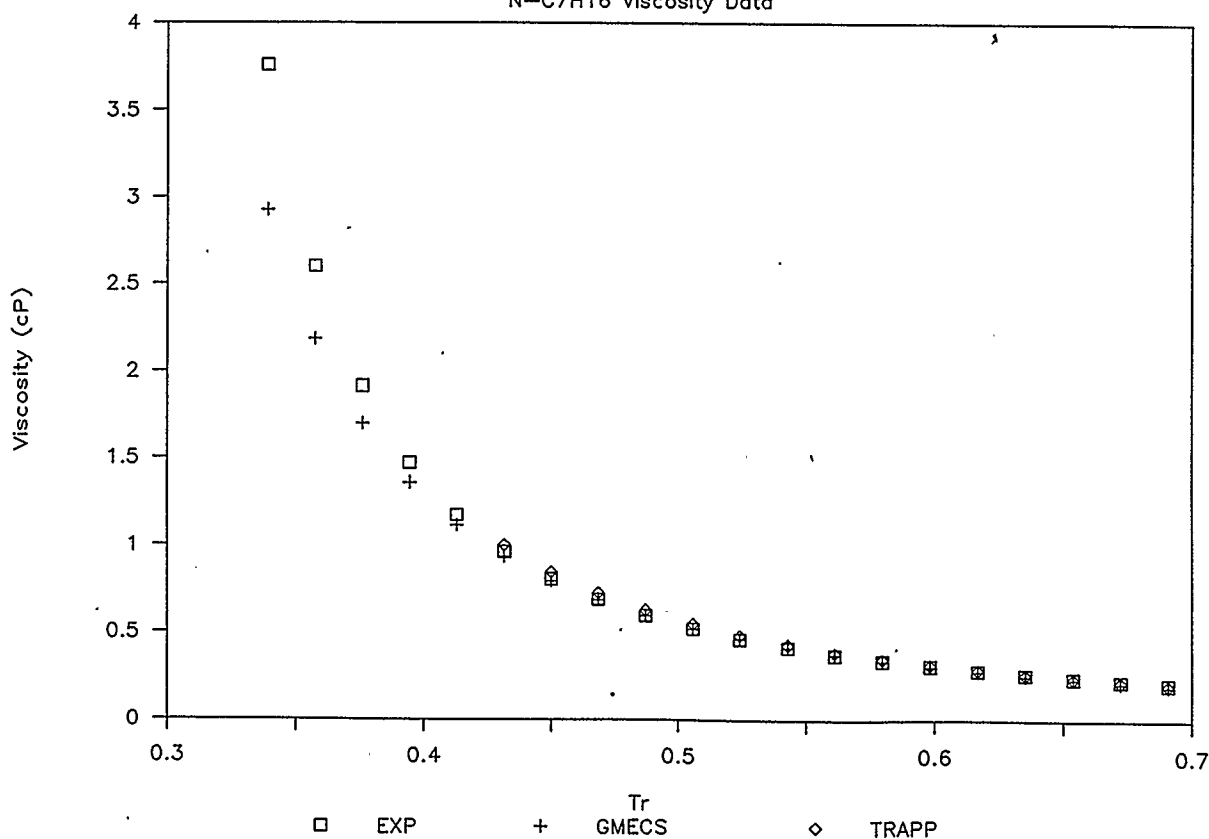


Table A-10
n-Octane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-50.00	0.3923	1.8500	1.7326	
101.325	-40.00	0.4099	1.4600	1.3990	
101.325	-30.00	0.4275	1.1790	1.1552	
101.325	-20.00	0.4450	0.9780	0.9717	1.0045
101.325	-10.00	0.4626	0.8270	0.8299	0.8588
101.325	0.00	0.4802	0.7104	0.7179	0.7428
101.325	10.00	0.4978	0.6184	0.6277	0.6489
101.325	20.00	0.5154	0.5450	0.5539	0.5718
101.325	30.00	0.5329	0.4850	0.4925	0.5077
101.325	40.00	0.5505	0.4355	0.4409	0.4537
101.325	50.00	0.5681	0.3935	0.3970	0.4078
101.325	60.00	0.5857	0.3576	0.3593	0.3684
101.325	70.00	0.6033	0.3264	0.3265	0.3343
101.325	80.00	0.6208	0.2995	0.2978	
101.325	90.00	0.6384	0.2759	0.2725	
101.325	100.00	0.6560	0.2547	0.2500	
101.325	110.00	0.6736	0.2359	0.2299	
101.325	120.00	0.6911	0.2188	0.2119	

Figure A-10

N-C8H18 Viscosity Data

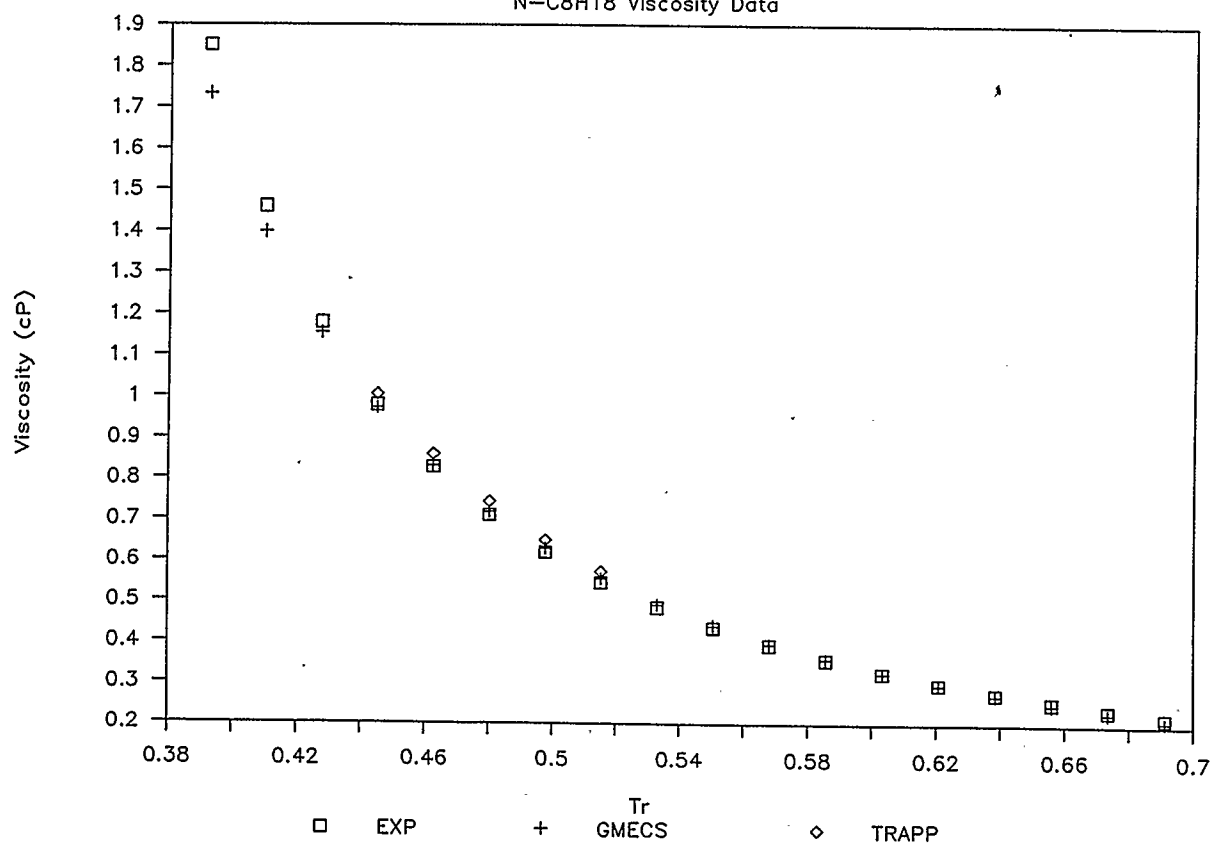


Table A-11
n-Nonane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-50.00	0.3753	2.9800	2.6683	
101.325	-40.00	0.3921	2.2300	2.0727	
101.325	-30.00	0.4090	1.7430	1.6576	
101.325	-20.00	0.4258	1.3990	1.3575	
101.325	-10.00	0.4426	1.1510	1.1336	1.1478
101.325	0.00	0.4594	0.9659	0.9622	0.9792
101.325	10.00	0.4762	0.8242	0.8278	0.8451
101.325	20.00	0.4931	0.7139	0.7205	0.7368
101.325	30.00	0.5099	0.6260	0.6332	0.6481
101.325	40.00	0.5267	0.5545	0.5611	0.5744
101.325	50.00	0.5435	0.4955	0.5009	0.5125
101.325	60.00	0.5603	0.4459	0.4499	0.4600
101.325	70.00	0.5771	0.4035	0.4062	0.4151
101.325	80.00	0.5940	0.3676	0.3685	0.3762
101.325	90.00	0.6108	0.3365	0.3357	0.3424
101.325	100.00	0.6276	0.3091	0.3069	
101.325	110.00	0.6444	0.2849	0.2814	
101.325	120.00	0.6612	0.2633	0.2587	
101.325	130.00	0.6781	0.2438	0.2383	
101.325	140.00	0.6949	0.2264	0.2200	

Figure A-11

N-C₉H₂₀ Viscosity Data

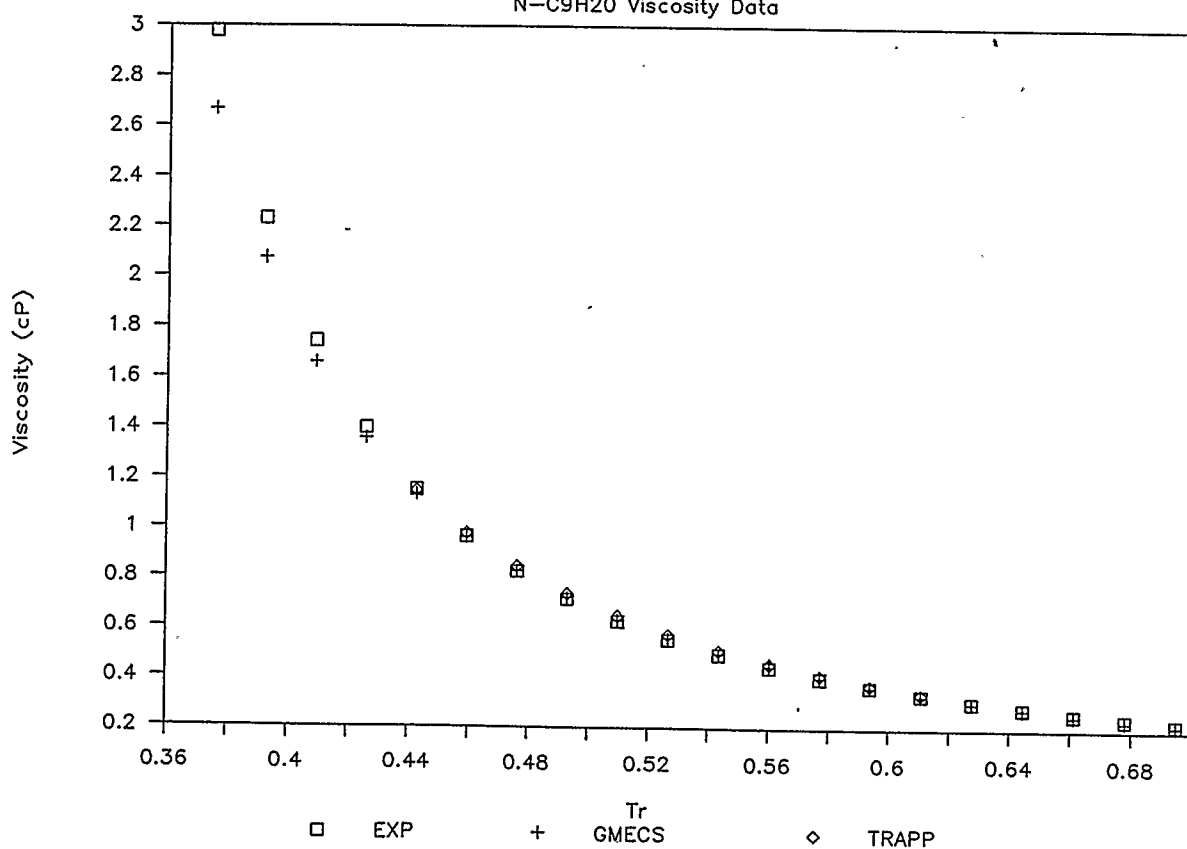


Table A-12
n-Decane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4099	1.9810	1.8693	
101.325	-10.00	0.4261	1.5850	1.5250	
101.325	0.00	0.4423	1.3000	1.2692	1.2681
101.325	10.00	0.4585	1.0870	1.0739	1.0806
101.325	20.00	0.4747	0.9256	0.9215	0.9317
101.325	30.00	0.4909	0.7994	0.8001	0.8113
101.325	40.00	0.5071	0.6989	0.7016	0.7128
101.325	50.00	0.5233	0.6174	0.6207	0.6311
101.325	60.00	0.5395	0.5501	0.5532	0.5625
101.325	70.00	0.5557	0.4936	0.4962	0.5044
101.325	80.00	0.5719	0.4463	0.4475	0.4547
101.325	90.00	0.5880	0.4056	0.4057	0.4119
101.325	100.00	0.6042	0.3704	0.3693	0.3746
101.325	110.00	0.6204	0.3398	0.3374	0.3419
101.325	120.00	0.6366	0.3128	0.3093	
101.325	130.00	0.6528	0.2887	0.2843	
101.325	140.00	0.6690	0.2675	0.2620	
101.325	150.00	0.6852	0.2482	0.2420	
101.325	160.00	0.7014	0.2306	0.2238	

Figure A-12

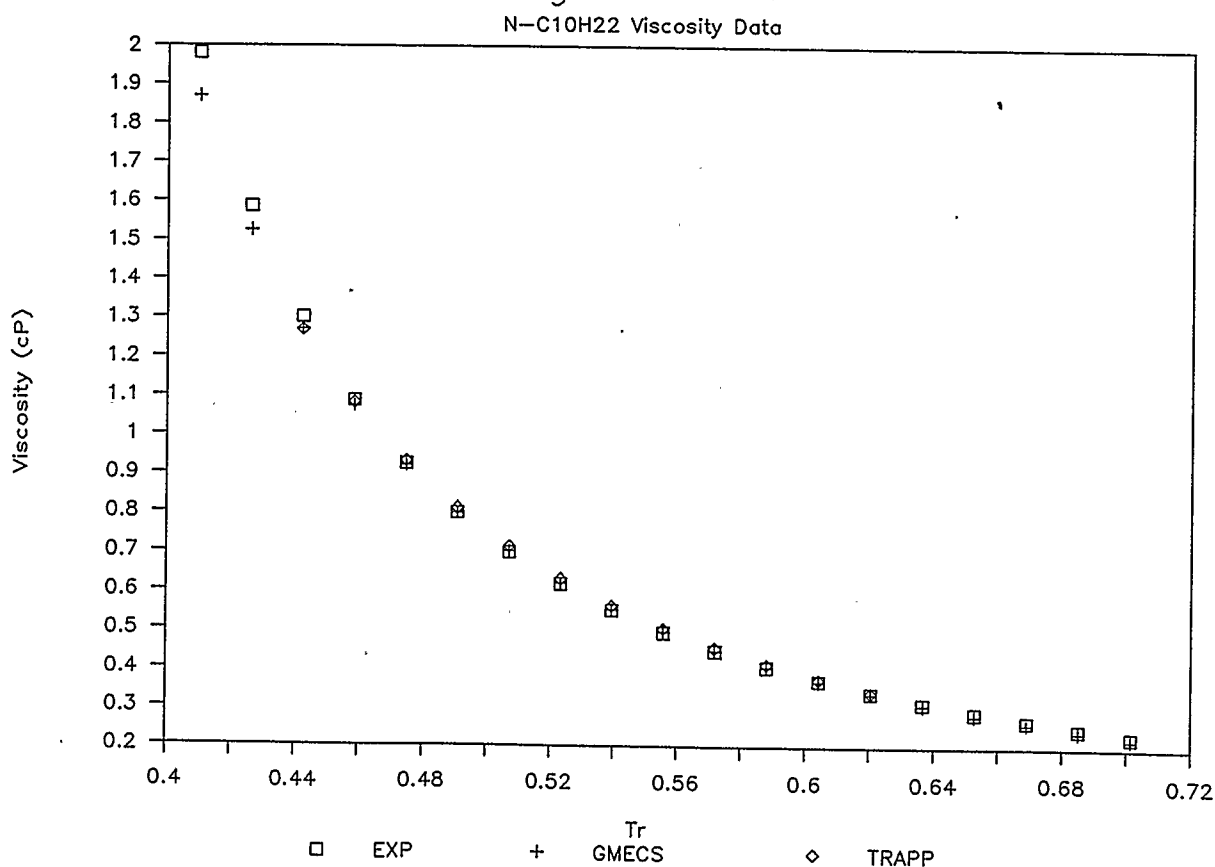


Table A-13
N-Undecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.3963	2.7710	2.5516	
101.325	-10.00	0.4119	2.1570	2.0320	
101.325	0.00	0.4276	1.7280	1.6571	1.6392
101.325	10.00	0.4433	1.4170	1.3783	1.3781
101.325	20.00	0.4589	1.1850	1.1654	1.1741
101.325	30.00	0.4746	1.0090	0.9992	1.0117
101.325	40.00	0.4902	0.8707	0.8669	0.8806
101.325	50.00	0.5059	0.7604	0.7598	0.7731
101.325	60.00	0.5216	0.6711	0.6717	0.6840
101.325	70.00	0.5372	0.5970	0.5984	0.6094
101.325	80.00	0.5529	0.5355	0.5365	0.5461
101.325	90.00	0.5685	0.4836	0.4838	0.4920
101.325	100.00	0.5842	0.4390	0.4384	0.4454
101.325	120.00	0.6155	0.3669	0.3646	0.3694
101.325	140.00	0.6468	0.3115	0.3074	
101.325	160.00	0.6781	0.2675	0.2618	
101.325	180.00	0.7094	0.2313	0.2247	

Figure A-13

N-C₁₁H₂₄ Viscosity Data

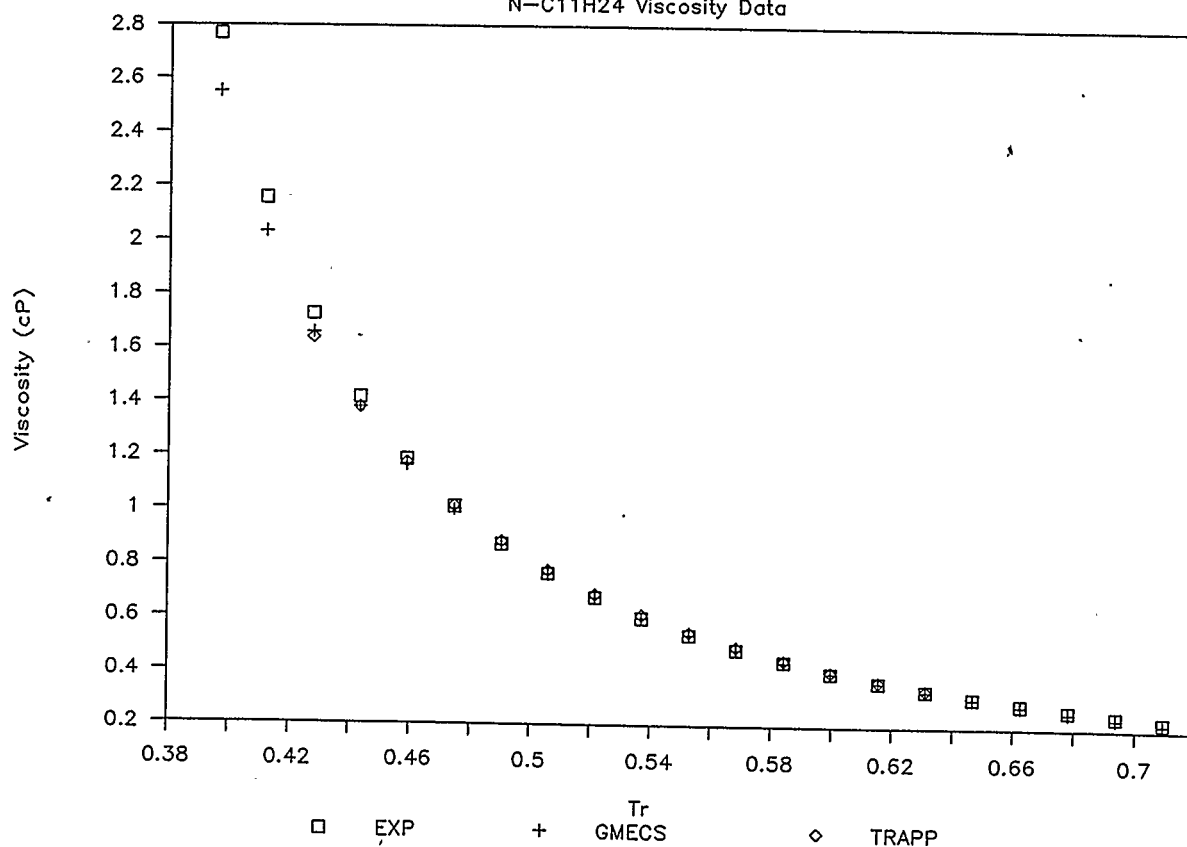


Table A-14
n-Dodecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	0.00	0.4145	2.2710	2.1446	
101.325	10.00	0.4301	1.8280	1.7527	1.7565
101.325	20.00	0.4453	1.5030	1.4601	1.4776
101.325	30.00	0.4605	1.2610	1.2361	1.2591
101.325	40.00	0.4757	1.0780	0.8669	1.0851
101.325	50.00	0.4909	0.9293	0.9210	0.9443
101.325	60.00	0.5061	0.8123	0.8076	0.8289
101.325	70.00	0.5213	0.7166	0.7143	0.7332
101.325	80.00	0.5365	0.6379	0.5984	0.6529
101.325	90.00	0.5517	0.5726	0.5710	0.5849
101.325	100.00	0.5668	0.5168	0.5150	0.4454
101.325	120.00	0.5973	0.4278	0.4252	0.4332
101.325	140.00	0.6276	0.3606	0.3565	0.3617
101.325	160.00	0.6580	0.3080	0.3025	
101.325	180.00	0.6884	0.2656	0.2591	
101.325	200.00	0.7188	0.2304	0.2235	

Figure A-14

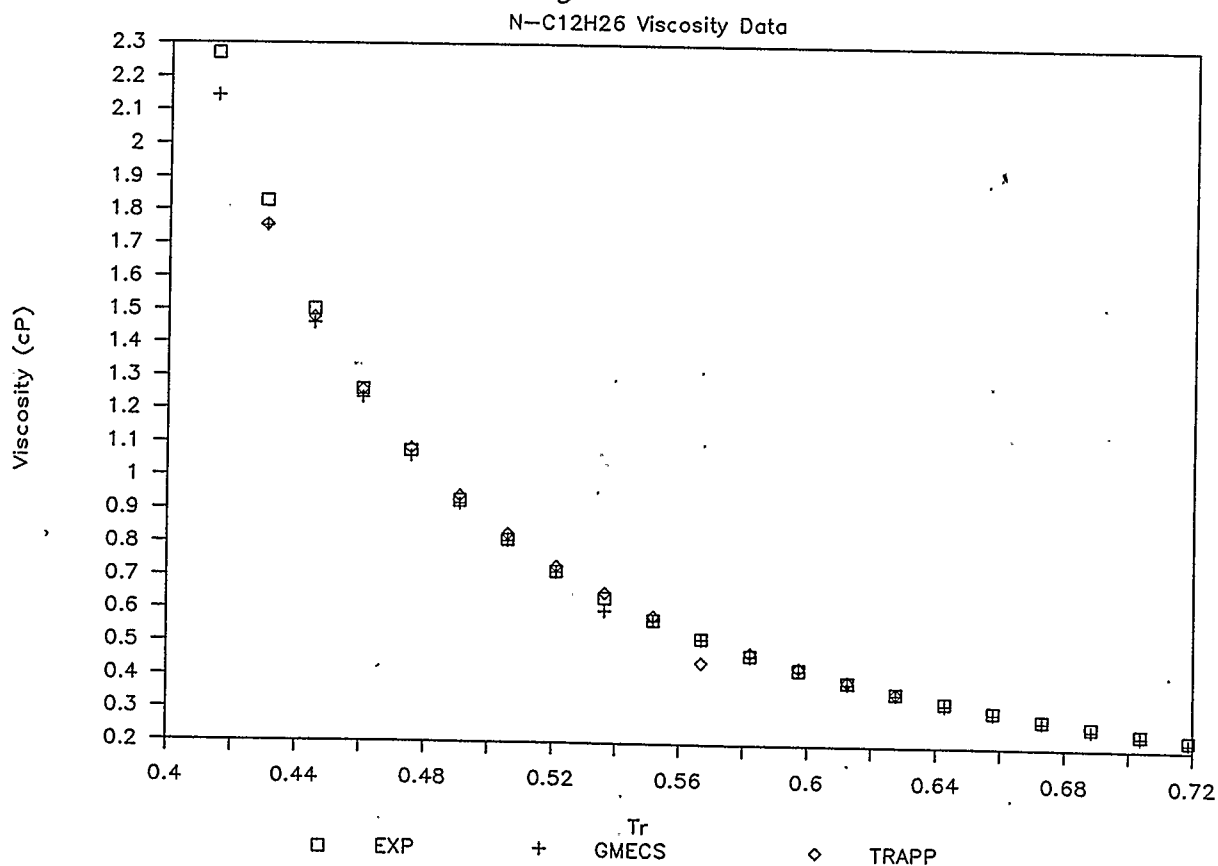


Table A-15
n-Tridecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	0.00	0.4038	2.9410	2.7411	
101.325	10.00	0.4185	2.3210	2.2013	
101.325	20.00	0.4333	1.8800	1.8066	1.8407
101.325	30.00	0.4481	1.5550	1.5100	1.5504
101.325	40.00	0.4629	1.3100	1.2817	1.3225
101.325	50.00	0.4777	1.1200	1.1023	1.1405
101.325	60.00	0.4925	0.9696	0.9588	0.9930
101.325	70.00	0.5073	0.8488	0.8421	0.8719
101.325	80.00	0.5221	0.7505	0.7458	0.7714
101.325	90.00	0.5367	0.6689	0.6653	0.6870
101.325	100.00	0.5517	0.6004	0.5974	0.6154
101.325	120.00	0.5812	0.4925	0.4894	0.5015
101.325	140.00	0.6108	0.4121	0.4080	0.4157
101.325	160.00	0.6404	0.3642	0.3448	0.3493
101.325	180.00	0.6699	0.3008	0.2945	
101.325	200.00	0.6995	0.2608	0.2537	
101.325	220.00	0.7291	0.2261	0.2198	

Figure A-15

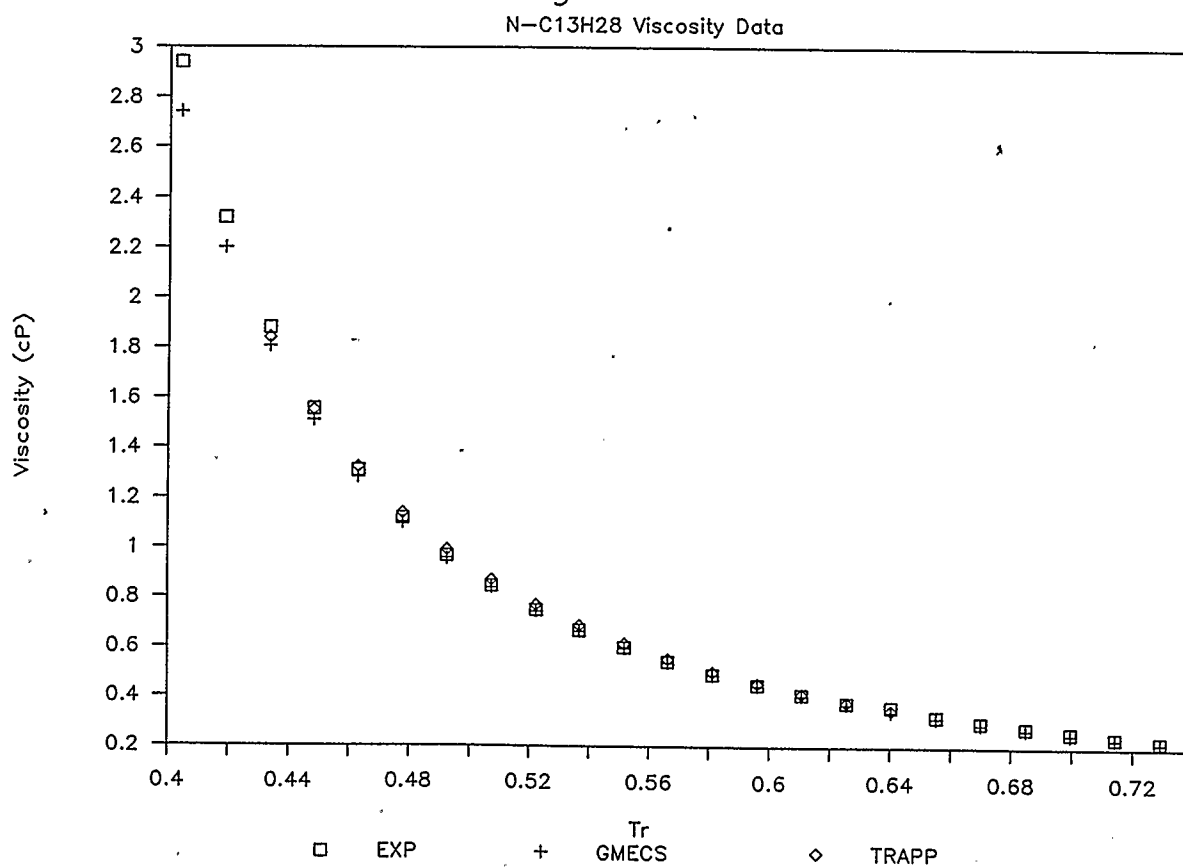


Table A-16
n-Tetradecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	10.00	0.4086	2.9310	2.7496	
101.325	20.00	0.4230	2.3350	2.2230	
101.325	30.00	0.4375	1.9040	1.8343	1.8853
101.325	40.00	0.4519	1.5850	1.5399	1.5916
101.325	50.00	0.4663	1.3410	1.3119	1.3600
101.325	60.00	0.4808	1.1510	1.1317	1.1745
101.325	70.00	0.4952	0.9990	0.9868	1.0238
101.325	80.00	0.5096	0.8772	0.8686	0.8998
101.325	90.00	0.5241	0.7772	0.7707	0.7966
101.325	100.00	0.5385	0.6937	0.6887	0.7098
101.325	120.00	0.5673	0.5637	0.5599	0.5732
101.325	140.00	0.5962	0.4682	0.4640	0.4716
101.325	160.00	0.6251	0.3954	0.3904	0.3939
101.325	180.00	0.6539	0.3385	0.3325	
101.325	200.00	0.6828	0.2926	0.2858	
101.325	220.00	0.7117	0.2539	0.2475	
101.325	240.00	0.7405	0.2211	0.2154	

Figure A-16

N-C14H30 Viscosity Data

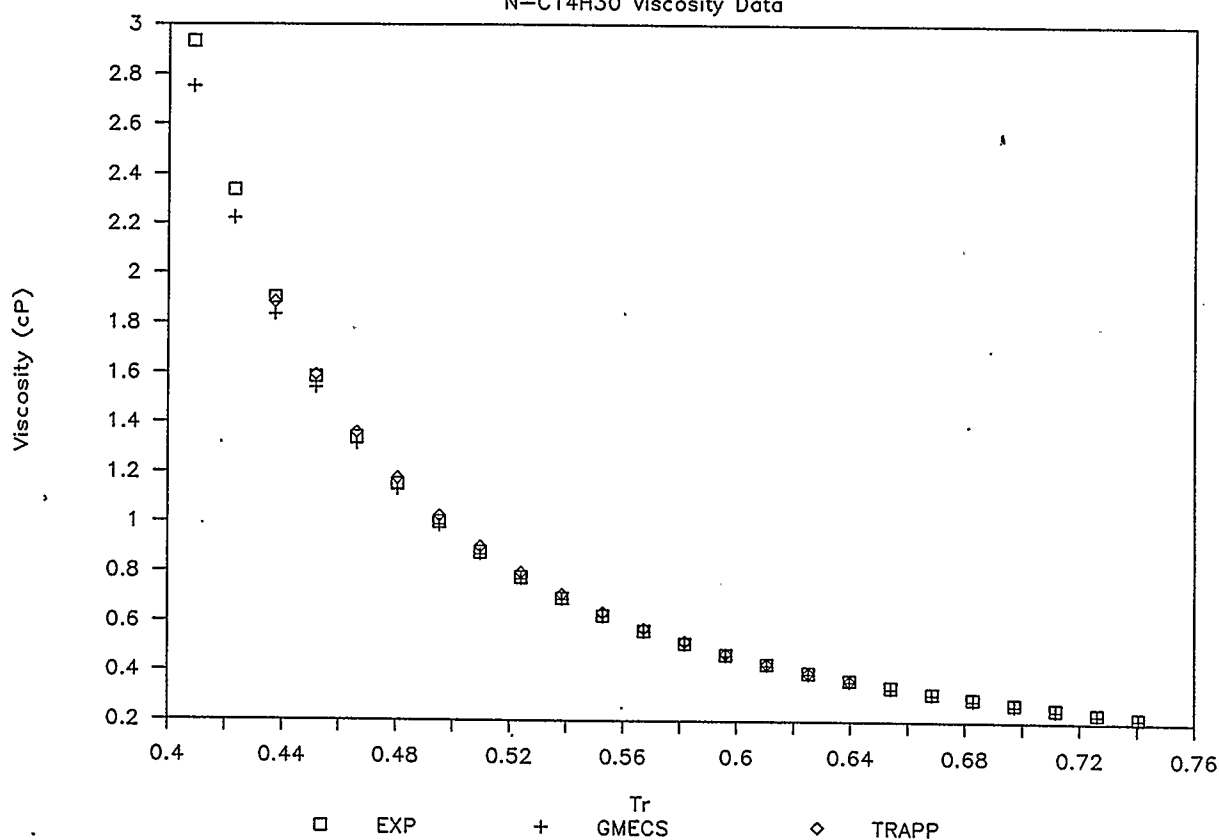


Table A-17

n-Pentadecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	10.00	0.4006	3.6520	3.3821	
101.325	20.00	0.4145	2.8630	2.6949	
101.325	30.00	0.4289	2.3030	2.1962	
101.325	40.00	0.4430	1.8940	1.8241	1.9471
101.325	50.00	0.4572	1.5860	1.5397	1.6457
101.325	60.00	0.4714	1.3490	1.3177	1.4073
101.325	70.00	0.4855	1.1630	1.1411	1.2160
101.325	80.00	0.4997	1.0140	0.9983	1.0603
101.325	90.00	0.5138	0.8926	0.8811	0.9320
101.325	100.00	0.5279	0.7925	0.7838	0.8252
101.325	120.00	0.5563	0.6384	0.6323	0.6590
101.325	140.00	0.5846	0.5264	0.5210	0.5372
101.325	160.00	0.6129	0.4424	0.4365	0.4453
101.325	180.00	0.6412	0.3770	0.3705	0.3741
101.325	200.00	0.6894	0.3251	0.3178	
101.325	220.00	0.6977	0.2819	0.2748	
101.325	240.00	0.7261	0.2457	0.2391	

Figure A-17

N-C15H32 Viscosity Data

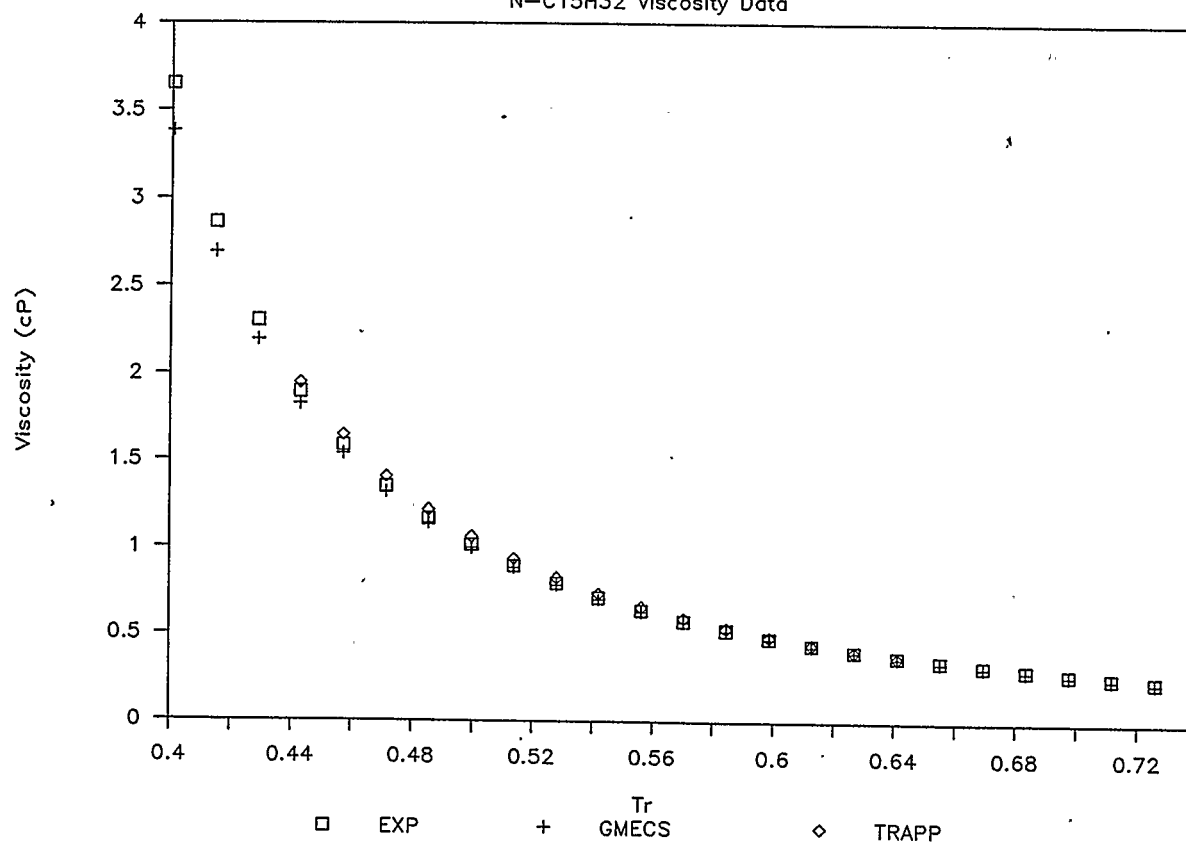


Table A-18
n-Hexadecane Viscosity Data

P(kPa)	T(°C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	20.00	0.4068	3.4740	3.2531	
101.325	30.00	0.4207	2.7580	2.6185	
101.325	40.00	0.4346	2.2430	2.1519	
101.325	50.00	0.4485	1.8600	1.7998	1.9721
101.325	60.00	0.4624	1.5680	1.5280	1.6705
101.325	70.00	0.4762	1.3420	1.3141	1.4312
101.325	80.00	0.4901	1.1620	1.1427	1.2385
101.325	90.00	0.5040	1.0180	1.0033	1.0812
101.325	100.00	0.5179	0.8992	0.8883	0.9513
101.325	120.00	0.5456	0.7181	0.7113	0.7516
101.325	140.00	0.5734	0.5882	0.5827	0.6073
101.325	160.00	0.6011	0.4915	0.4860	0.4998
101.325	180.00	0.6289	0.4174	0.4111	0.4174
101.325	200.00	0.6566	0.3586	0.3518	0.3527
101.325	220.00	0.6844	0.3107	0.3037	
101.325	240.00	0.7122	0.2710	0.2641	
101.325	260.00	0.7399	0.2370	0.2309	
101.325	280.00	0.7677	0.2090	0.2026	

Figure A-18

N-C16H34 Viscosity Data

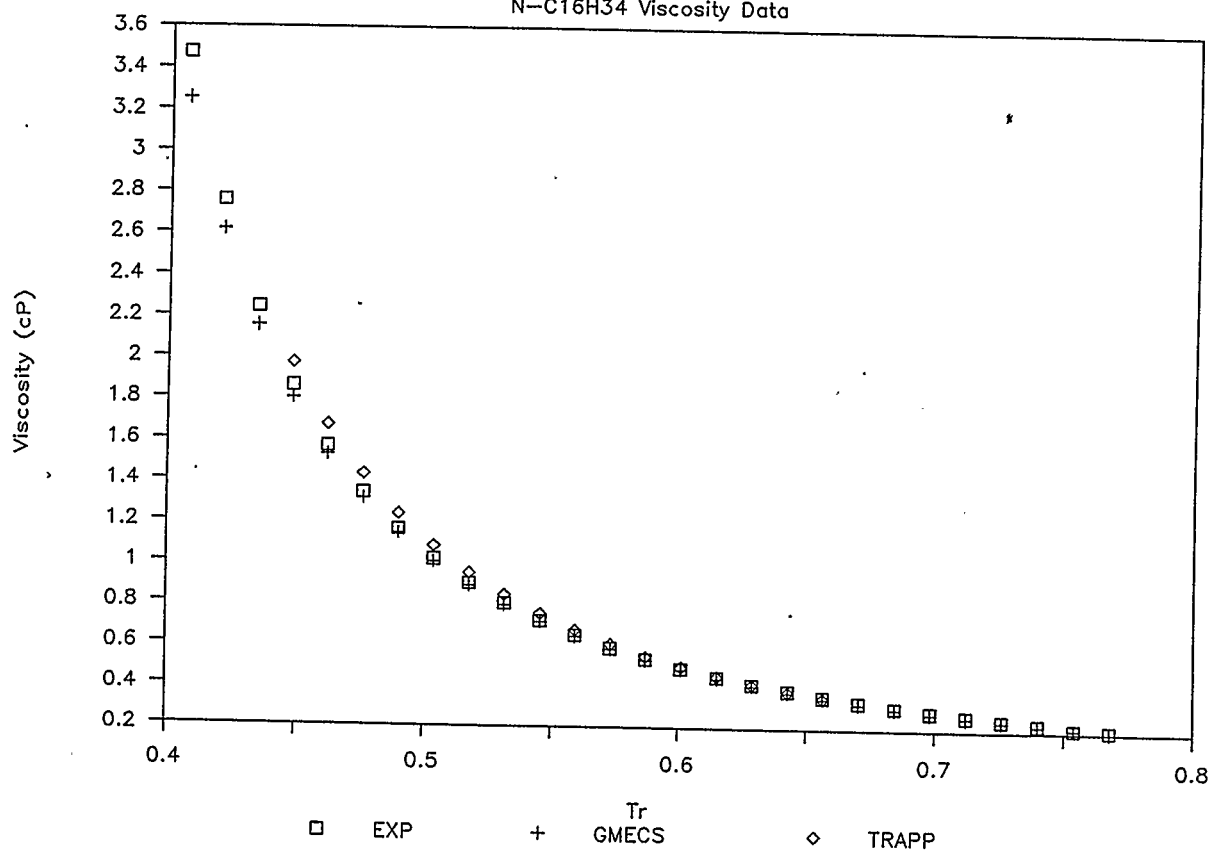


Table A-19
n-Heptadecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	30.00	0.4134	3.2860	3.0971	
101.325	40.00	0.4270	2.6420	2.5191	
101.325	50.00	0.4406	2.1700	2.0882	
101.325	60.00	0.4543	1.8150	1.7592	1.9339
101.325	70.00	0.4679	1.5410	1.5028	1.6439
101.325	80.00	0.4815	1.3260	1.2992	1.4126
101.325	90.00	0.4952	1.1550	1.1349	1.2255
101.325	100.00	0.5088	1.0150	1.0003	1.0722
101.325	120.00	0.5361	0.8040	0.7950	0.8388
101.325	140.00	0.5634	0.6540	0.6475	0.6723
101.325	160.00	0.5906	0.5438	0.5377	0.5496
101.325	180.00	0.6179	0.4597	0.4533	0.4565
101.325	200.00	0.6452	0.3939	0.3869	0.3841
101.325	220.00	0.6725	0.3407	0.3335	
101.325	240.00	0.6997	0.2969	0.2897	
101.325	260.00	0.7270	0.2600	0.2531	
101.325	280.00	0.7543	0.2290	0.2223	

Figure A-19

N-C₁₇H₃₆ Viscosity Data

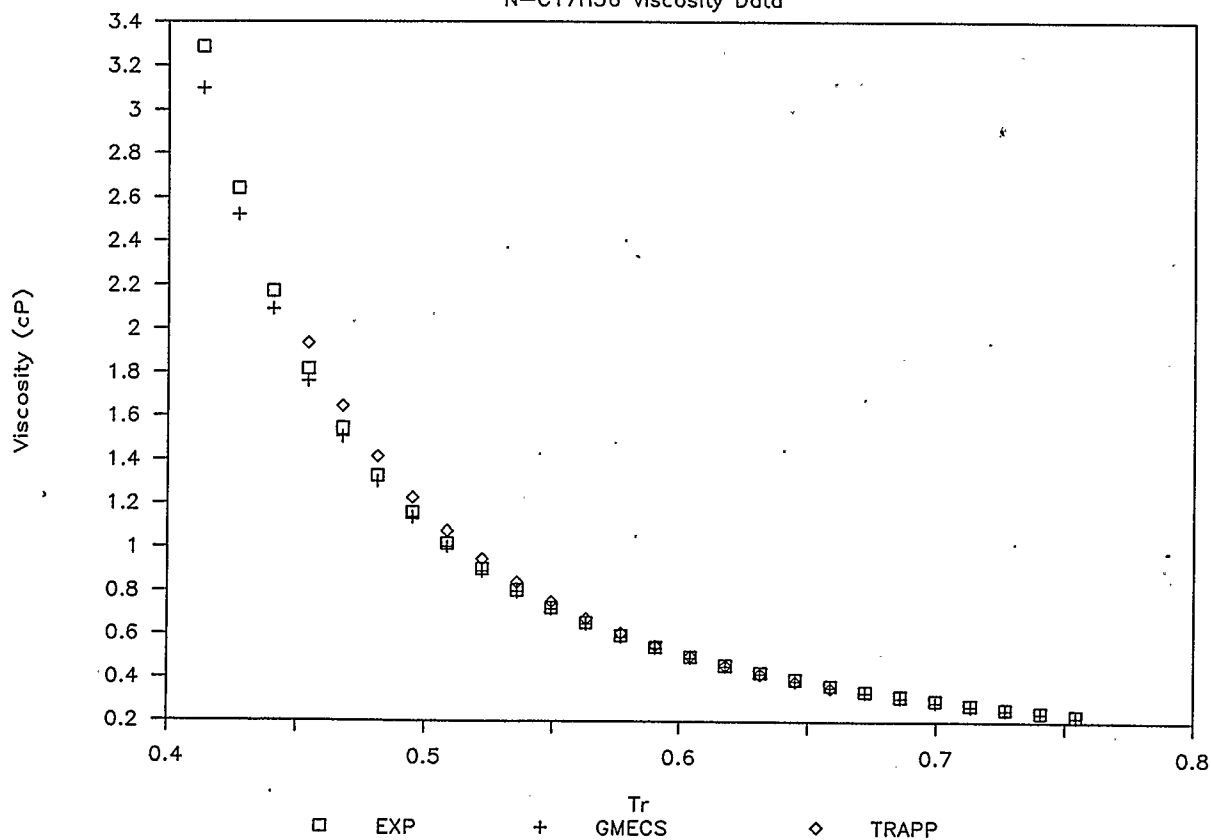


Table A-20
n-Octadecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	30.00	0.4052	3.8790	3.6410	
101.325	40.00	0.4185	3.0840	2.9307	
101.325	50.00	0.4319	2.5080	2.4076	
101.325	60.00	0.4453	2.0810	2.0125	
101.325	70.00	0.4586	1.7550	1.7074	1.8838
101.325	80.00	0.4720	1.5010	1.4673	1.6064
101.325	90.00	0.4854	1.2990	1.2750	1.3840
101.325	100.00	0.4987	1.1370	1.1187	1.2034
101.325	120.00	0.5255	0.8930	0.8824	0.9315
101.325	140.00	0.5522	0.7220	0.7145	0.7401
101.325	160.00	0.5789	0.5970	0.5906	0.6007
101.325	180.00	0.6056	0.5020	0.4962	0.4960
101.325	200.00	0.6324	0.4300	0.4224	0.4153
101.325	220.00	0.6591	0.3710	0.3633	0.3518
101.325	240.00	0.6858	0.3230	0.3152	
101.325	260.00	0.7126	0.2800	0.2753	
101.325	280.00	0.7393	0.2500	0.2417	
101.325	300.00	0.7660	0.2200	0.2130	

Figure A-20

N-C18H38 Viscosity Data

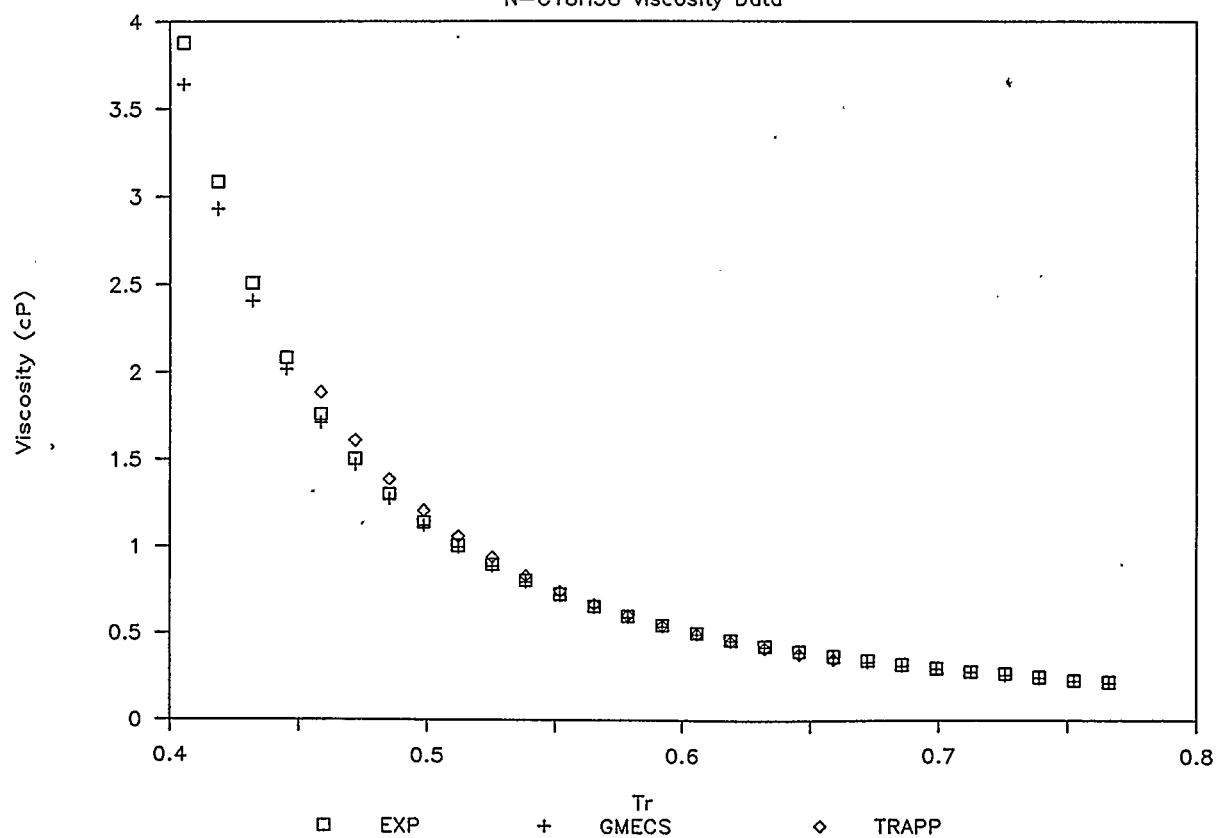


Table A-21
n-Nonadecane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	40.00	0.4142	3.5770	3.3311	
101.325	50.00	0.4274	2.8820	2.7151	
101.325	60.00	0.4407	2.3720	2.2541	
101.325	70.00	0.4539	1.9860	1.9011	
101.325	80.00	0.4671	1.6880	1.6253	1.7910
101.325	90.00	0.4804	1.4540	1.4059	1.5331
101.325	100.00	0.4936	1.2650	1.2286	1.3252
101.325	120.00	0.5200	0.9860	0.9627	1.0154
101.325	140.00	0.5465	0.7930	0.7755	0.8000
101.325	160.00	0.5730	0.6520	0.6384	0.6447
101.325	180.00	0.5994	0.5470	0.5347	0.5292
101.325	200.00	0.6259	0.4670	0.4541	0.4409
101.325	220.00	0.6523	0.4010	0.3899	0.3719
101.325	240.00	0.6788	0.3490	0.3379	
101.325	260.00	0.7052	0.3100	0.2949	
101.325	280.00	0.7317	0.2700	0.2588	
101.325	300.00	0.7581	0.2400	0.2282	
101.325	320.00	0.7846	0.2100	0.2018	

Figure A-21

N-C19H40 Viscosity Data

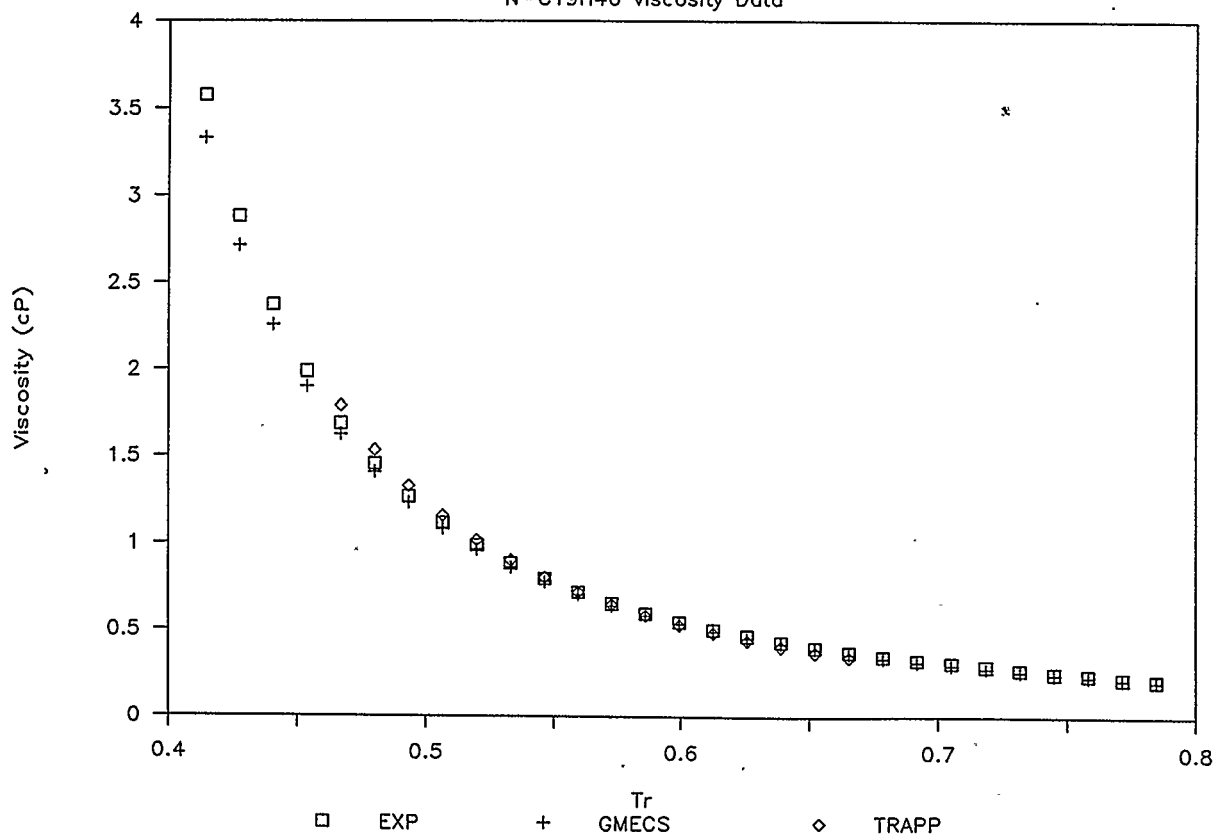


Table A-22
n-Eicosane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	40.00	0.4083	4.1440	3.8263	
101.325	50.00	0.4213	3.3060	3.0920	
101.325	60.00	0.4343	2.6980	2.5480	
101.325	70.00	0.4474	2.2420	2.1350	
101.325	80.00	0.4604	1.8940	1.8149	
101.325	90.00	0.4735	1.6220	1.5621	2.0902
101.325	100.00	0.4865	1.4060	1.3591	1.7850
101.325	120.00	0.5126	1.0880	1.0571	1.3394
101.325	140.00	0.5387	0.8680	0.8467	1.0371
101.325	160.00	0.5647	0.7110	0.6940	0.8236
101.325	180.00	0.5908	0.5940	0.5792	0.6676
101.325	200.00	0.6169	0.5040	0.4906	0.5504
101.325	220.00	0.6430	0.4340	0.4204	0.4601
101.325	240.00	0.6690	0.3760	0.3637	0.3890
101.325	260.00	0.6951	0.3300	0.3172	
101.325	280.00	0.7212	0.2900	0.2783	
101.325	300.00	0.7473	0.2600	0.2453	
101.325	320.00	0.7733	0.2300	0.2171	

Figure A-22

N-C20H42 Viscosity Data

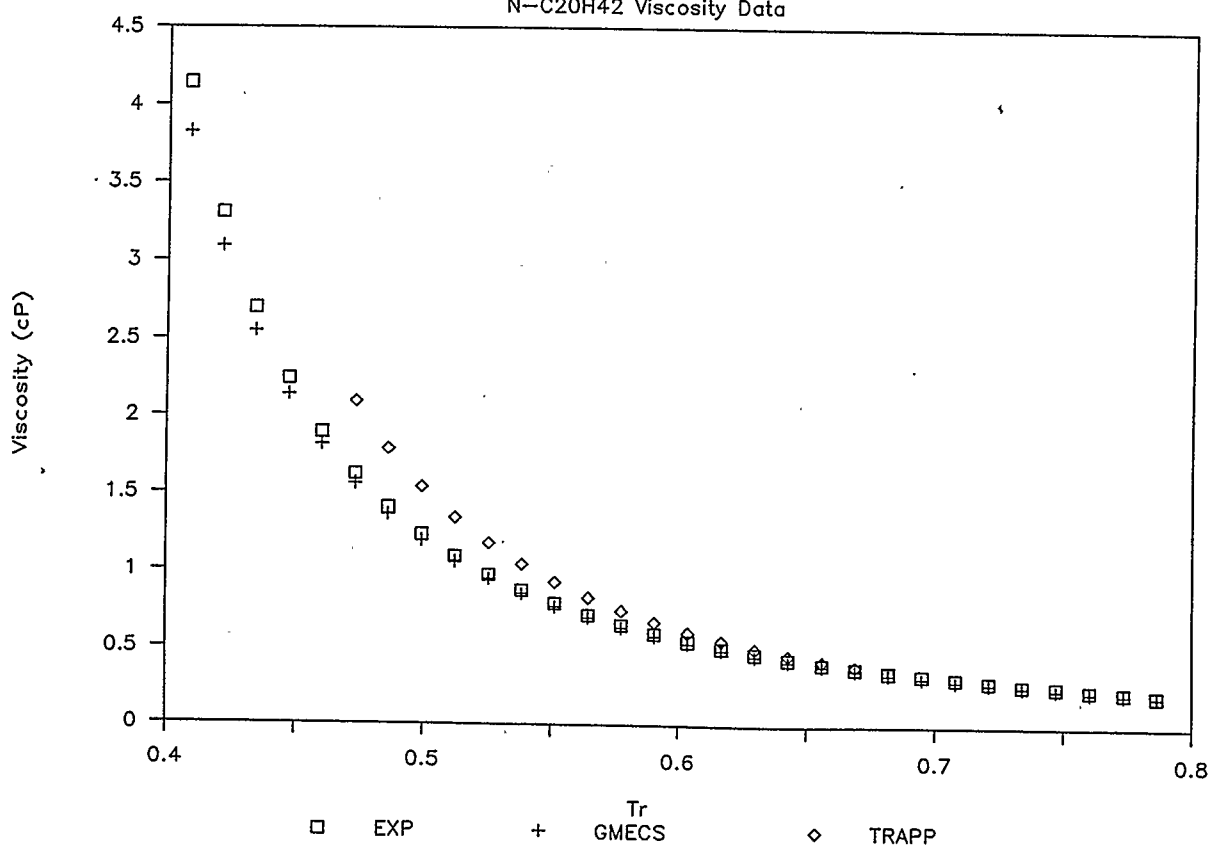


Table A-23
Ethene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.3250	-160.00	0.4007	0.5100	0.5248	
101.3250	-150.00	0.4361	0.3900	0.4038	0.3884
101.3250	-140.00	0.4715	0.3100	0.3214	0.3116
101.325	-130.00	0.5069	0.2600	0.2621	0.2564
101.325	-120.00	0.5423	0.2100	0.2175	0.2151
101.325	-110.00	0.5777	0.1800	0.1828	0.1830
101.325	-100.00	0.6131	0.1500	0.1550	

Figure A-23

C2H4 Viscosity Data

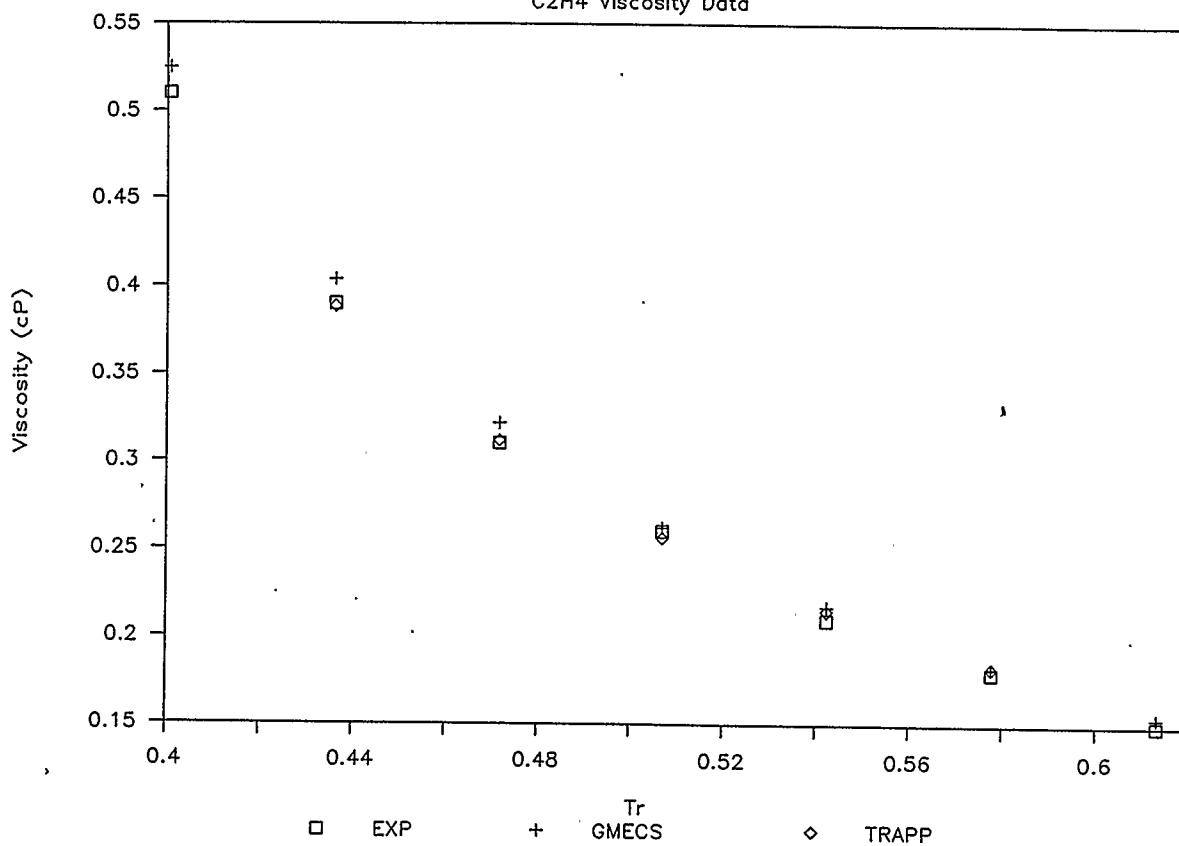


Table A-24
Propene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-170.00	0.2827	3.5300	2.8085	
101.325	-160.00	0.3101	1.9600	1.7512	
101.325	-150.00	0.3375	1.2900	1.2031	1.2816
101.325	-140.00	0.3649	0.9100	0.8834	0.9461
101.325	-130.00	0.3924	0.6800	0.6801	0.7300
101.325	-120.00	0.4198	0.5400	0.5420	0.5824
101.325	-110.00	0.4472	0.4400	0.4434	0.4770
101.325	-100.00	0.4746	0.3700	0.3699	

Figure A-24

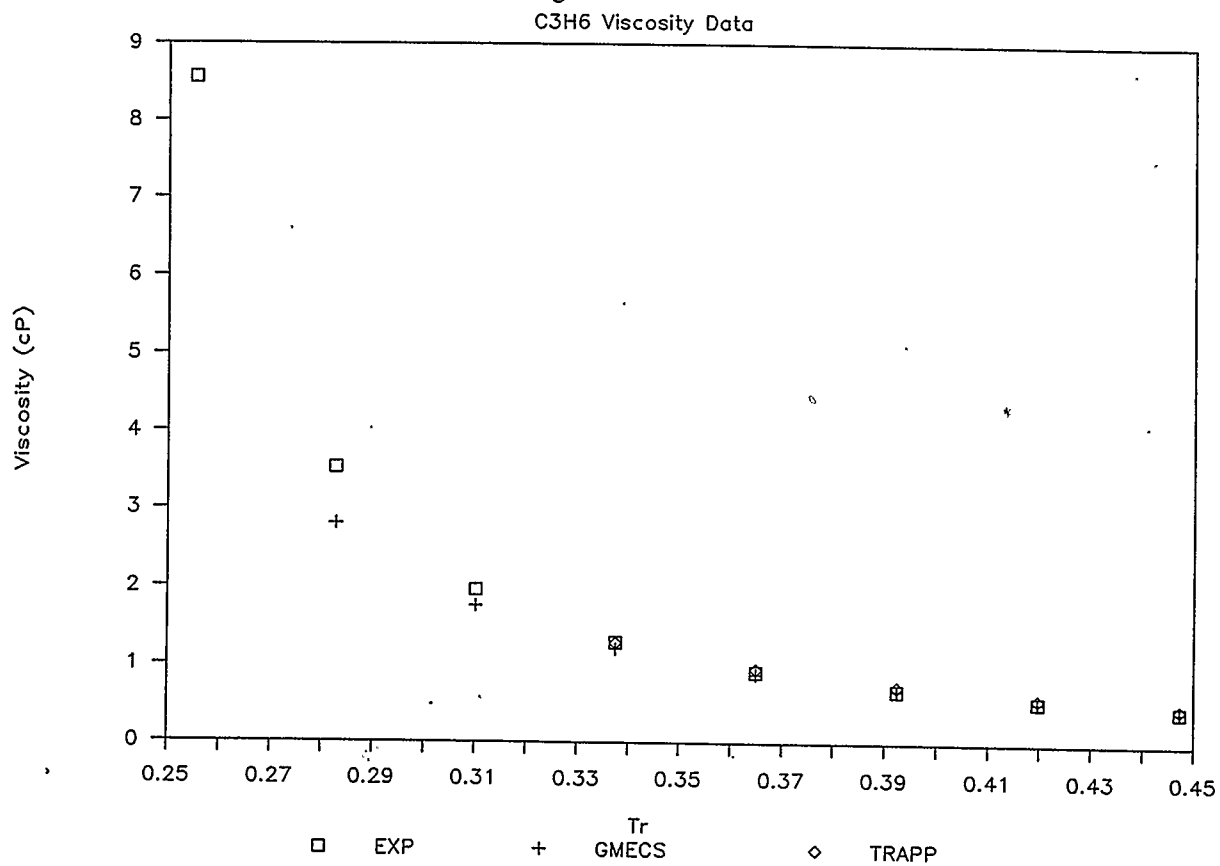


Table A-25
1-Butene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-100.00	0.4127	0.6400	0.6484	
101.325	-90.00	0.4365	0.5300	0.5367	0.6083
101.325	-80.00	0.4603	0.4500	0.4522	0.5120
101.325	-70.00	0.4842	0.3900	0.3866	0.4376
101.325	-60.00	0.5079	0.3400	0.3343	0.3787
101.325	-50.00	0.5318	0.3000	0.2917	0.3311
101.325	-40.00	0.5556	0.2600	0.2565	

Figure A-25

1-C4H8 Viscosity Data

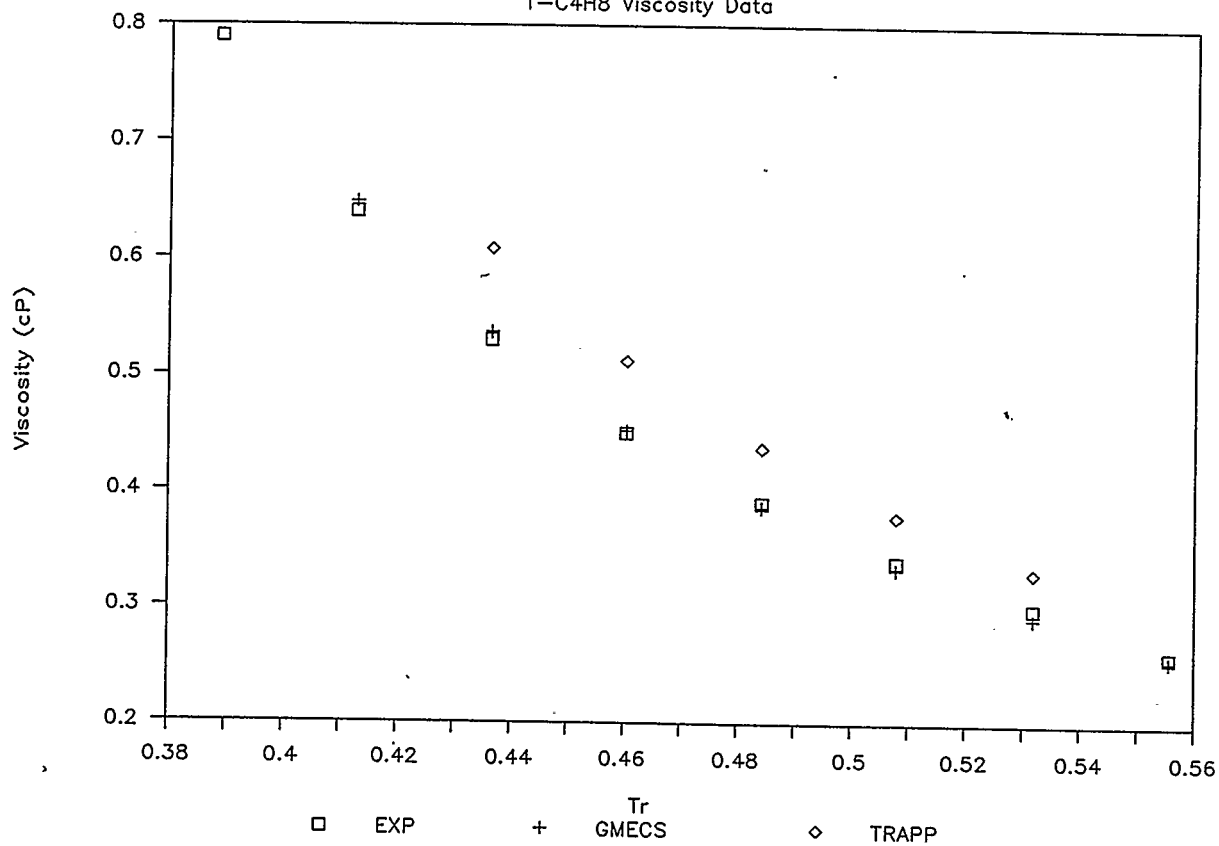


Table A-26
1-Pentene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	Trapp
101.325	-90.00	0.3941	0.8500		
101.325	-80.00	0.4156	0.7000	0.7038	1.0205
101.325	-70.00	0.4372	0.5900	0.5904	0.8492
101.325	-60.00	0.4586	0.5000	0.5030	0.7185
101.325	-50.00	0.4802	0.4300	0.4341	0.6165
101.325	-40.00	0.5017	0.3800	0.3786	0.5352
101.325	-30.00	0.5232	0.3300	0.3329	0.4692
101.325	-20.00	0.5448	0.3000	0.2949	0.4148
101.325	-10.00	0.5662	0.2700	0.2627	
101.325	0.00	0.5878	0.2400	0.2351	

Figure A-26
1-C₅H₁₀ Viscosity Data

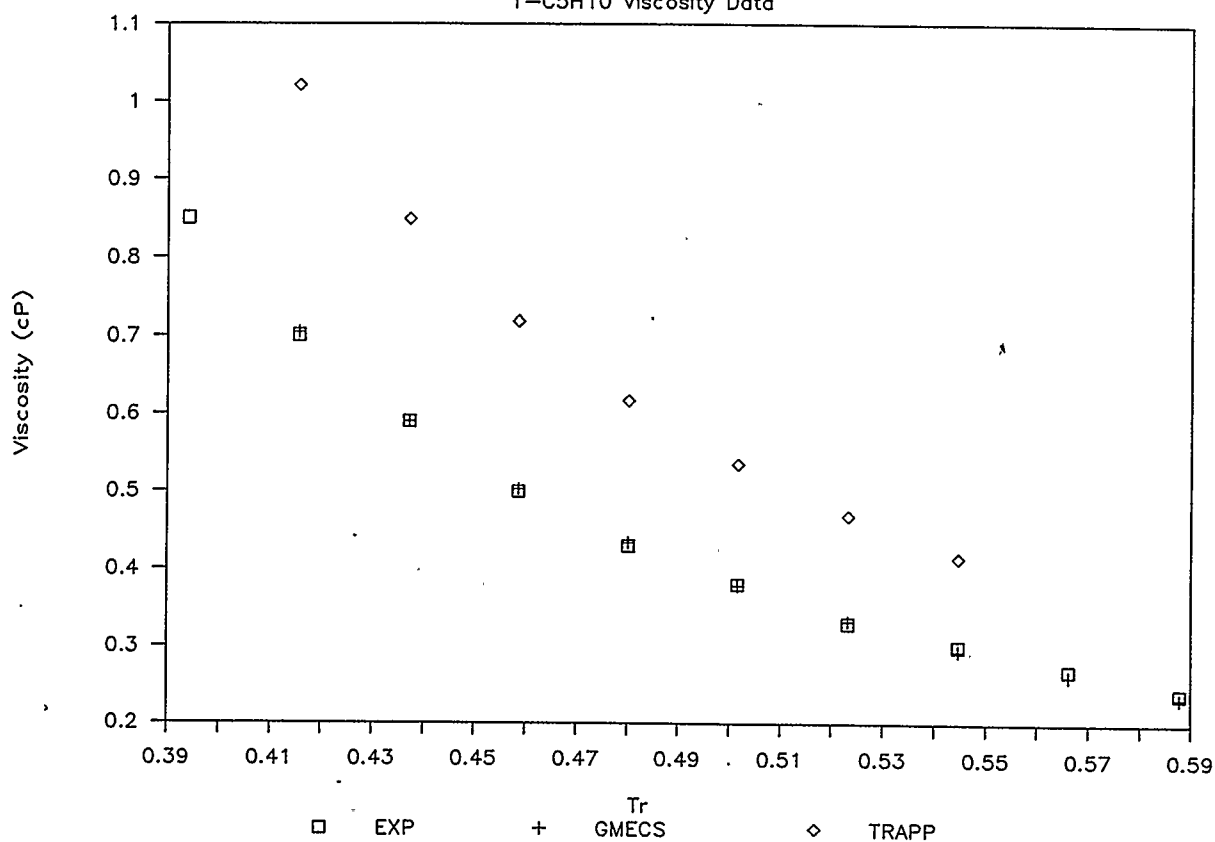


Table A-27
1-Hexene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-50.00	0.4428	0.6300	0.6344	0.7688
101.325	-40.00	0.4626	0.5400	0.5465	0.6566
101.325	-30.00	0.4824	0.4700	0.4759	0.5678
101.325	-20.00	0.5023	0.4200	0.4184	0.4961
101.325	-10.00	0.5221	0.3700	0.3706	0.4373
101.325	0.00	0.5420	0.3300	0.3304	0.3885
101.325	10.00	0.5618	0.2900	0.2962	0.3474
101.325	20.00	0.5816	0.2600	0.2668	0.3124
101.325	30.00	0.6015	0.2400	0.2411	0.2823
101.325	40.00	0.6213	0.2200	0.2187	
101.325	50.00	0.6412	0.2000	0.1987	
101.325	60.00	0.6610	0.1900	0.1809	

Figure A-27

1-C₆H₁₂ Viscosity Data

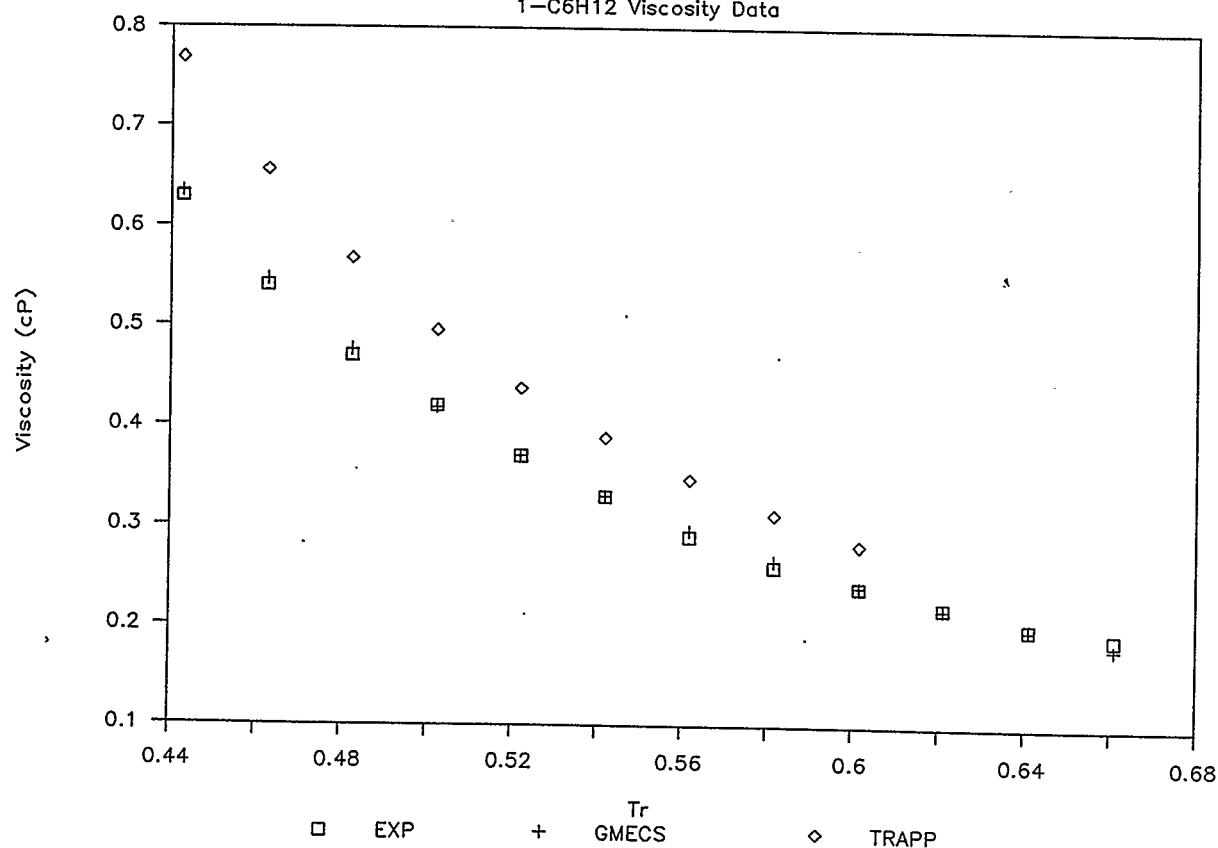


Table A-28
Cyclopentane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4947	0.7200	0.7415	0.4885
101.325	-10.00	0.5142	0.6290	0.6467	0.4348
101.325	0.00	0.5338	0.5530	0.5692	0.3896
101.325	10.00	0.5534	0.4910	0.5048	0.3512
101.325	20.00	0.5729	0.4380	0.4507	0.3182
101.325	30.00	0.5924	0.3930	0.4046	
101.325	40.00	0.6119	0.3550	0.3649	
101.325	50.00	0.6315	0.3220	0.3304	

Figure A-28

Cyclo-C5 Viscosity Data

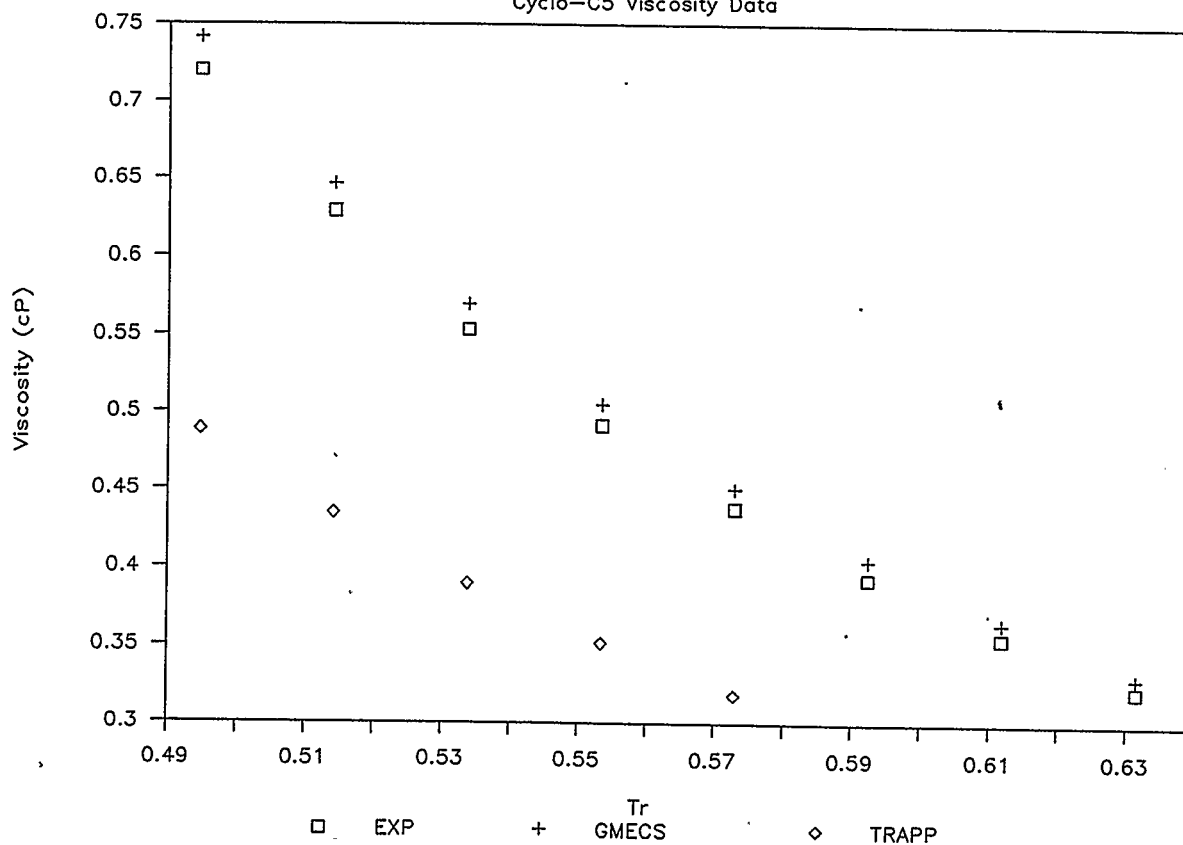


Table A-29
Methylcyclopentane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4752	0.8600	0.8065	0.5856
101.325	-10.00	0.4939	0.7430	0.7007	0.5172
101.325	0.00	0.5127	0.6480	0.6149	0.4603
101.325	10.00	0.5315	0.5700	0.5440	0.4125
101.325	20.00	0.5503	0.5050	0.4847	0.3718
101.325	30.00	0.5690	0.4510	0.4346	0.3369
101.325	40.00	0.5878	0.4040	0.3916	0.3065
101.325	50.00	0.6066	0.3640	0.3544	
101.325	60.00	0.6254	0.3290	0.3220	
101.325	70.00	0.6441	0.2990	0.2935	

Figure A-29

Methylcyclo-C5 Viscosity Data

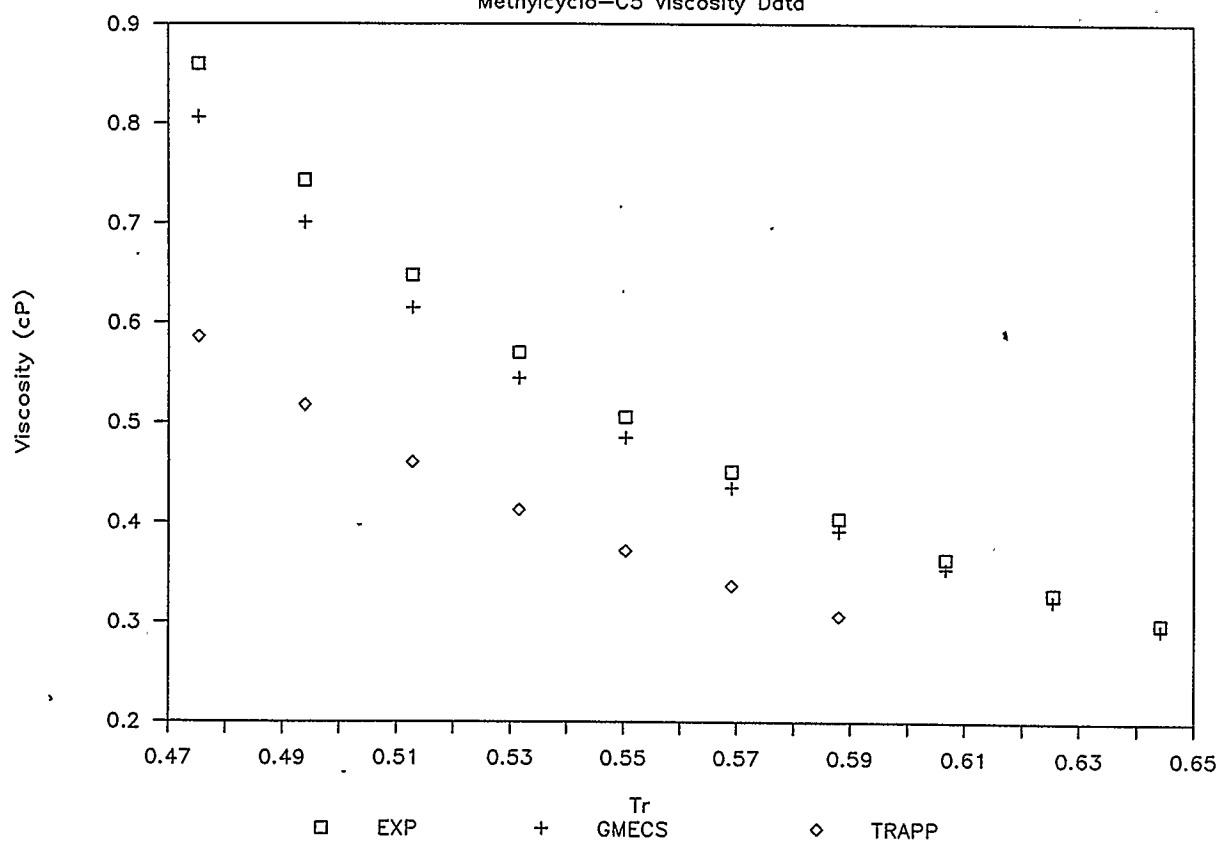


Table A-30
Ethylcyclopentane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4157	0.9600	0.9884	0.8125
101.325	-10.00	0.4321	0.8270	0.8507	0.7084
101.325	0.00	0.4485	0.7220	0.7405	0.6235
101.325	10.00	0.4649	0.6370	0.6509	0.5533
101.325	20.00	0.4814	0.5650	0.5768	0.4945
101.325	30.00	0.4978	0.5050	0.5148	0.4447
101.325	40.00	0.5142	0.4550	0.4622	0.4021
101.325	50.00	0.5306	0.4110	0.4171	0.4021
101.325	60.00	0.5470	0.3750	0.3781	0.3332
101.325	70.00	0.5635	0.3420	0.3441	
101.325	80.00	0.5799	0.3200	0.3141	
101.325	90.00	0.5963	0.2900	0.2876	
101.325	100.00	0.6127	0.2700	0.2640	

Figure A-30
Ethylcyclo-C5 Viscosity Data

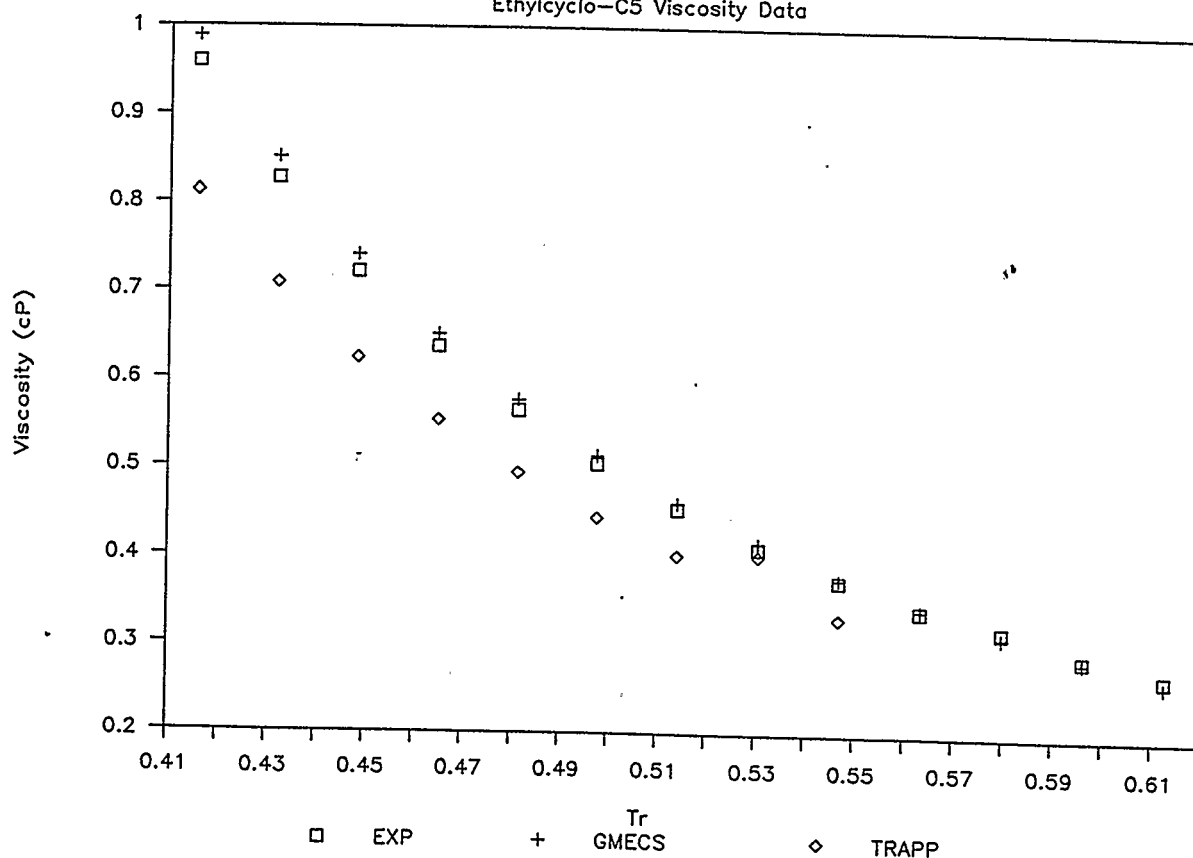


Table A-31
N-Propylcyclopentane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4246	1.2400	1.2346	
101.325	-10.00	0.4414	1.0500	1.0493	0.9679
101.325	0.00	0.4582	0.8950	0.9038	0.8394
101.325	10.00	0.4749	0.7770	0.7872	0.7351
101.325	20.00	0.4917	0.6800	0.6923	0.6494
101.325	30.00	0.5085	0.6020	0.6138	0.5780
101.325	40.00	0.5252	0.5380	0.5480	0.5179
101.325	50.00	0.5420	0.4870	0.4922	0.4666
101.325	60.00	0.5588	0.4430	0.4445	0.4226
101.325	70.00	0.5756	0.4060	0.4032	0.3845
101.325	80.00	0.5923	0.3800	0.3671	0.3512
101.325	90.00	0.6091	0.3500	0.3354	
101.325	100.00	0.6259	0.3300	0.3074	

Figure A-31

n-Propylcyclo-C5 Viscosity Data

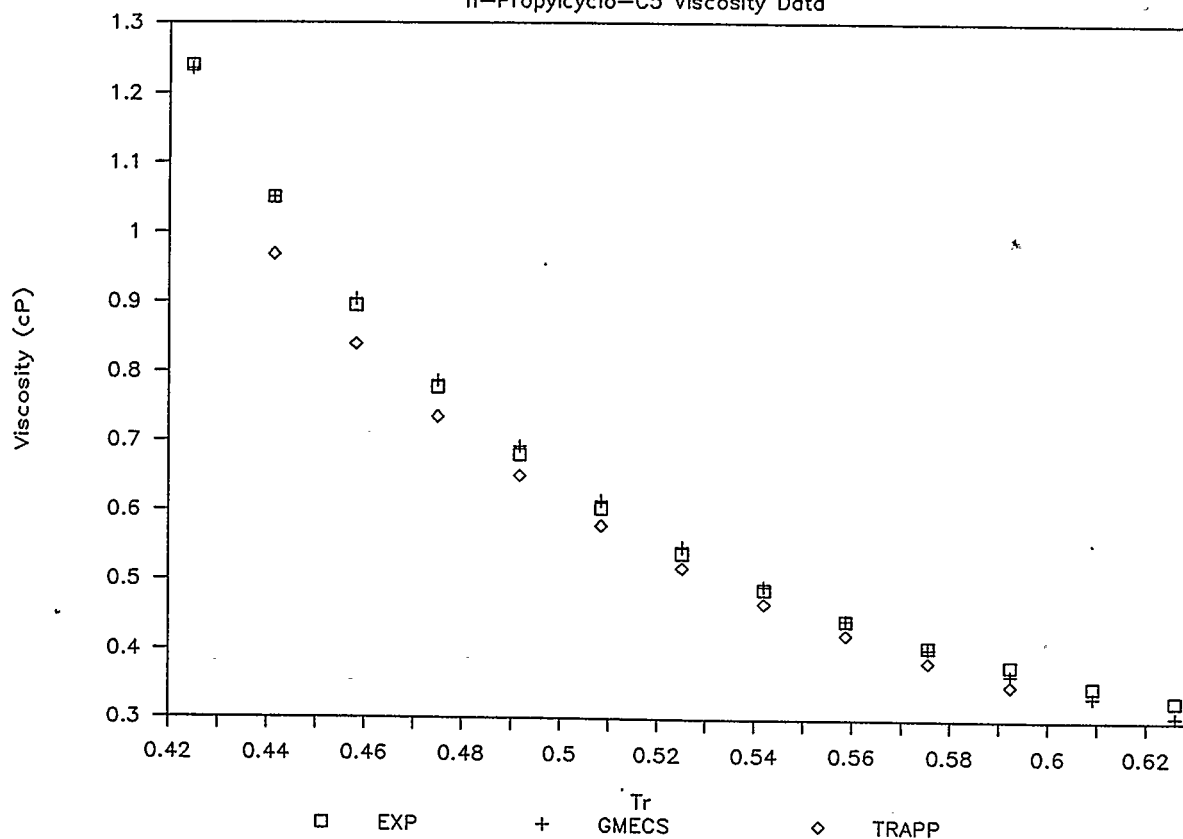


Table A-32
Cyclohexane Viscosity Data

P(kPa)	T(C)	Tr	-Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	10.00	0.5116	1.1760	1.0795	0.4615
101.325	20.00	0.5296	0.9770	0.9091	0.4159
101.325	30.00	0.5477	0.8240	0.7752	0.3767
101.325	40.00	0.5658	0.7020	0.6680	0.3429
101.325	50.00	0.5838	0.6040	0.5806	0.3134
101.325	60.00	0.6019	0.5260	0.5085	
101.325	70.00	0.6199	0.4630	0.4481	
101.325	80.00	0.6380	0.4100	0.3969	

Figure A-32

Cyclo-C6 Viscosity Data

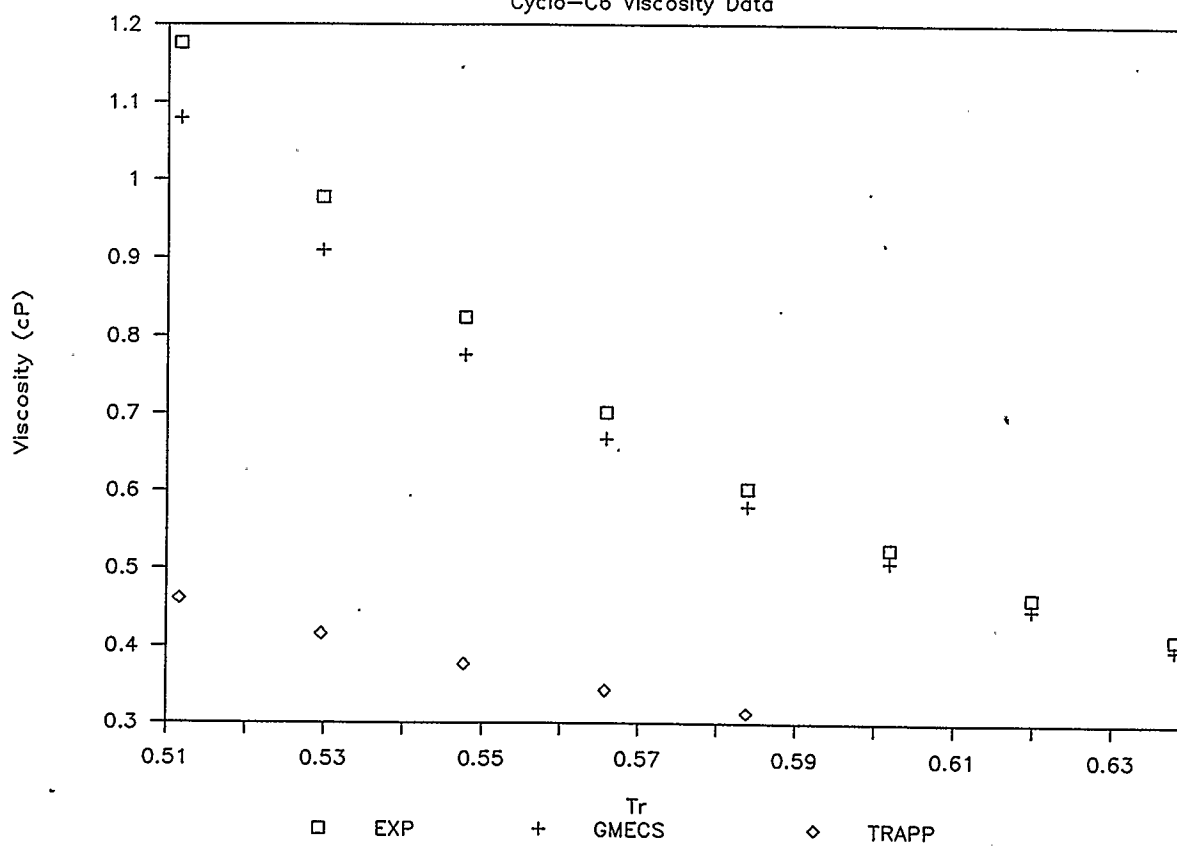


Table A-33
Methylcyclohexane Viscosity Data
Viscosity (cP)

P(kPa)	T(C)	Tr	Exp.	GMECS	TRAPP
101.325	-20.00	0.4424	1.4100	1.6305	
101.325	-10.00	0.4599	1.1800	1.3369	0.6617
101.325	0.00	0.4774	0.9900	1.1160	0.5849
101.325	10.00	0.4948	0.8470	0.9455	0.5210
101.325	20.00	0.5123	0.7329	0.8111	0.4673
101.325	30.00	0.5298	0.6390	0.7031	0.4216
101.325	40.00	0.5473	0.5620	0.6150	0.3823
101.325	50.00	0.5647	0.4990	0.5419	0.3483
101.325	60.00	0.5822	0.4450	0.4806	0.3185
101.325	70.00	0.5997	0.3990	0.4286	0.2924
101.325	80.00	0.6172	0.3600	0.3840	
101.325	90.00	0.6346	0.3300	0.3454	
101.325	100.00	0.6521	0.3000	0.3116	

Figure A-33

Methylcyclo-C6 Viscosity Data

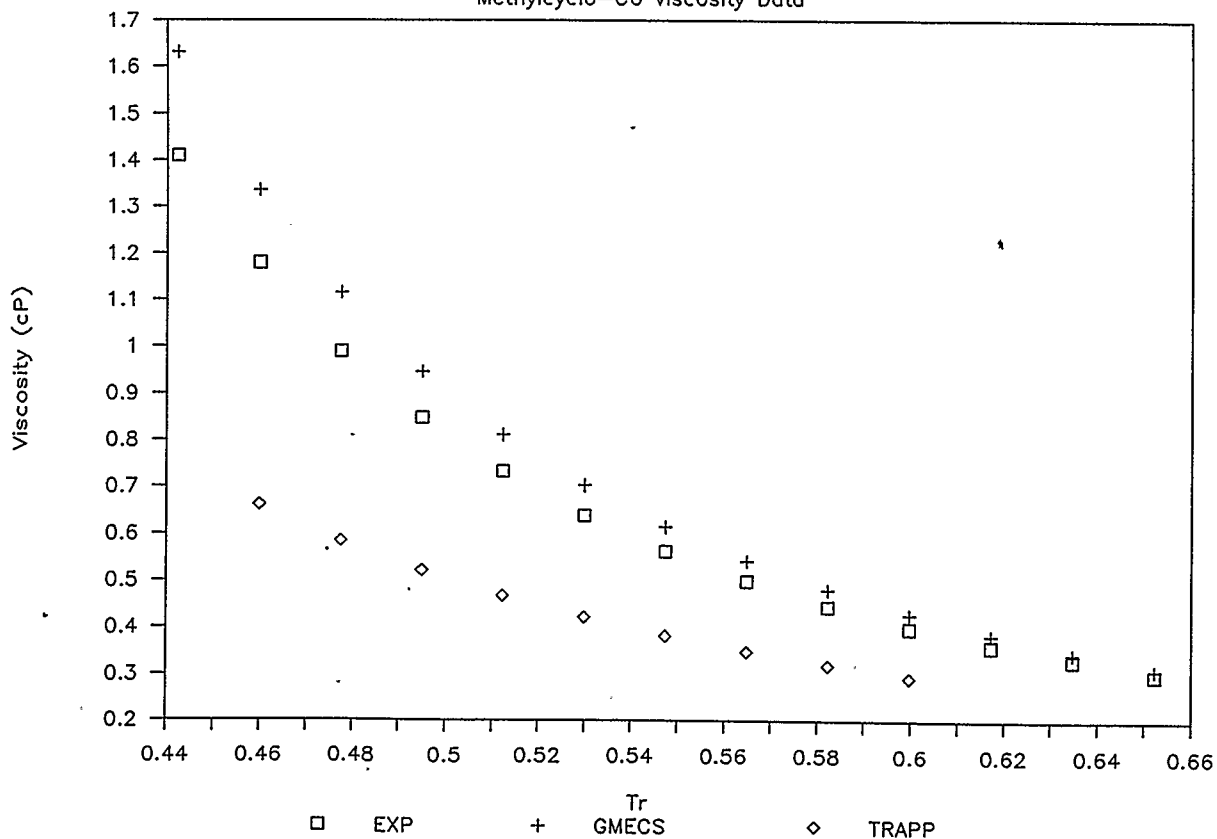


Table A-34
Ethylcyclohexane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4157	1.6300	1.4859	
101.325	-10.00	0.4321	1.3520	1.2399	0.8112
101.325	0.00	0.4485	1.1390	1.0510	0.7114
101.325	10.00	0.4649	0.9730	0.9028	0.6294
101.325	20.00	0.4814	0.8400	0.7841	0.5611
101.325	30.00	0.4978	0.7350	0.6875	0.5036
101.325	40.00	0.5143	0.6490	0.6077	0.4547
101.325	50.00	0.5306	0.5790	0.5409	0.4127
101.325	60.00	0.5470	0.5210	0.4844	0.3763
101.325	70.00	0.5635	0.4740	0.4360	0.3445
101.325	80.00	0.5799	0.4300	0.3942	0.3165
101.325	90.00	0.5963	0.4000	0.3578	0.2917
101.325	100.00	0.6127	0.3700	0.3258	

Figure A-34

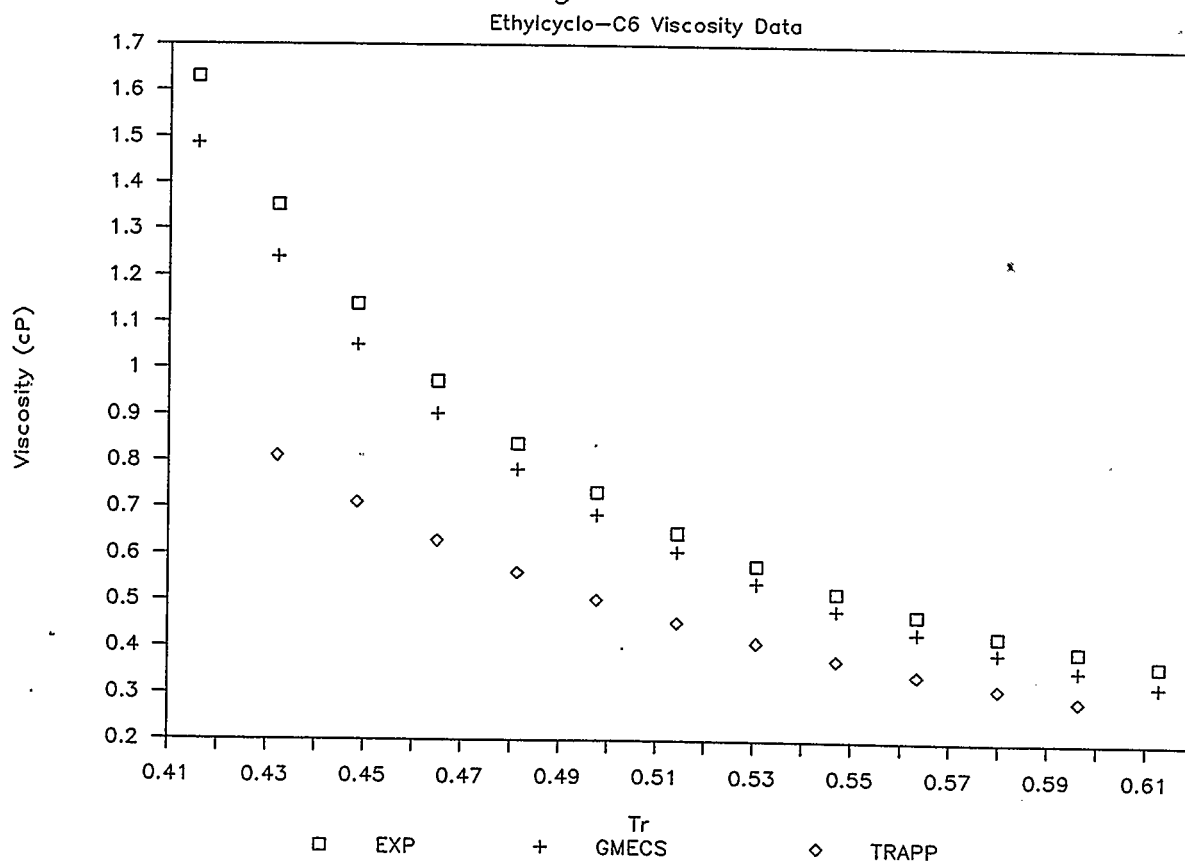


Table A-35
N-Propylcyclohexane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.3962	2.0900	1.9515	
101.325	-10.00	0.4118	1.7000	1.6065	0.9389
101.325	0.00	0.4275	1.4040	1.3466	0.8162
101.325	10.00	0.4431	1.1780	1.1460	0.7166
101.325	20.00	0.4588	1.0030	0.9878	0.6346
101.325	30.00	0.4744	0.8670	0.8608	0.5662
101.325	40.00	0.4901	0.7580	0.7570	0.5086
101.325	50.00	0.5057	0.6700	0.6711	0.4595
101.325	60.00	0.5214	0.5990	0.5991	0.4173
101.325	70.00	0.5370	0.5400	0.5380	0.3807
101.325	80.00	0.5526	0.4900	0.4856	0.3488
101.325	90.00	0.5683	0.4500	0.4403	0.3207
101.325	100.00	0.5839	0.4200	0.4008	0.2958

Figure A-35

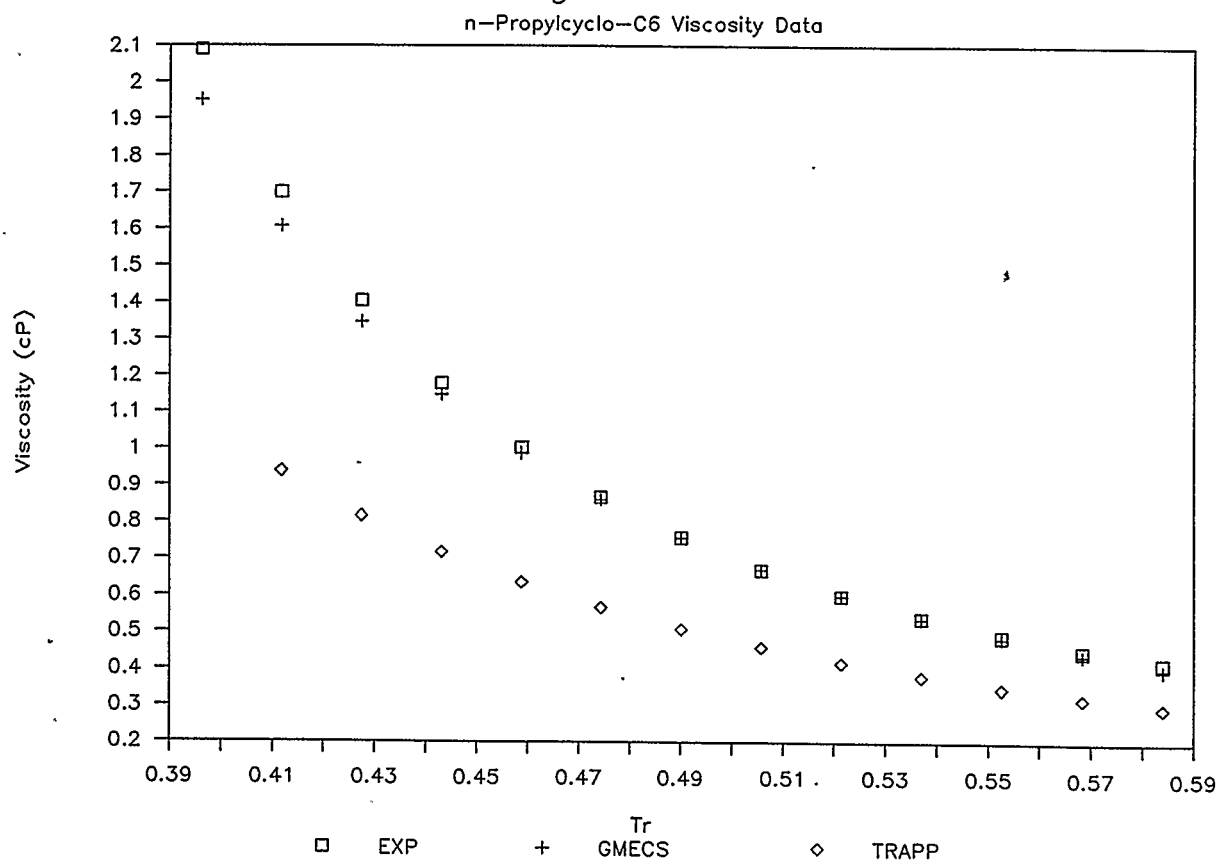


Table A-36
N-Butylcyclohexane Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.3795	2.9300	2.9710	2.4498
101.325	-10.00	0.3945	2.3400	2.3554	2.0435
101.325	0.00	0.4095	1.9000	1.9129	1.7302
101.325	10.00	0.4245	1.5690	1.5851	1.4840
101.325	20.00	0.4395	1.3100	1.3356	1.2870
101.325	30.00	0.4545	1.1110	1.1414	1.1271
101.325	40.00	0.4695	0.9520	0.9873	0.9954

Figure A-36

n-Butylcyclo-C6 Viscosity Data

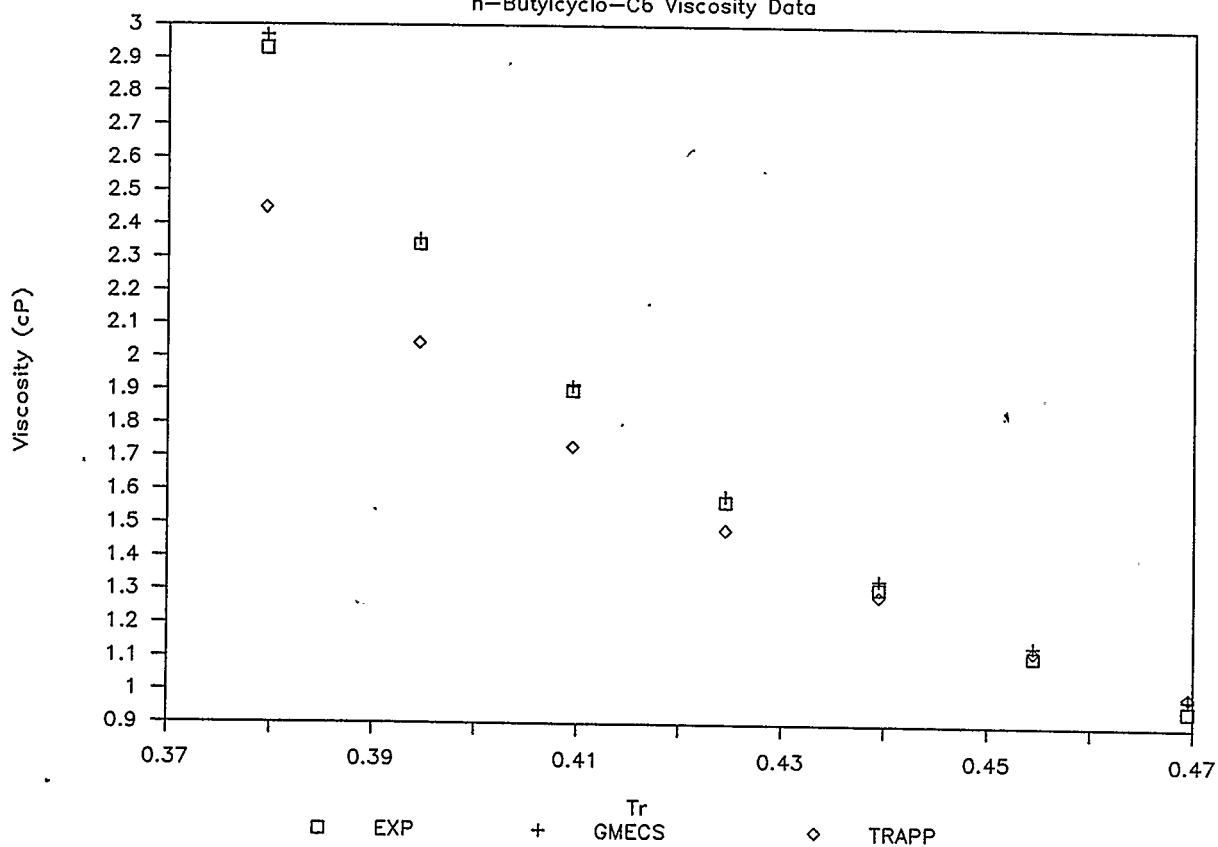


Table A-37
Benzene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	10.00	0.5037	0.7574	0.7051	0.5250
101.325	20.00	0.5215	0.6428	0.6199	0.4726
101.325	30.00	0.5393	0.5604	0.5489	0.4278
101.325	40.00	0.5570	0.4908	0.4892	0.3892
101.325	50.00	0.5748	0.4347	0.4382	0.3555
101.325	60.00	0.5926	0.3890	0.3944	
101.325	70.00	0.6104	0.3500	0.3563	
101.325	80.00	0.6282	0.3170	0.3229	
300.000	90.00	0.6459	0.2900	0.2940	0.2559
400.000	100.00	0.6638	0.2620	0.2680	0.2373
600.000	120.00	0.6994	0.2180	0.2237	0.2051
800.000	140.00	0.7349	0.1840	0.1873	0.1781
1000.000	160.00	0.7705	0.1520	0.1566	0.1550
1400.000	180.00	0.8061	0.1350	0.1305	0.1353

Figure A-37

Benzene Viscosity Data

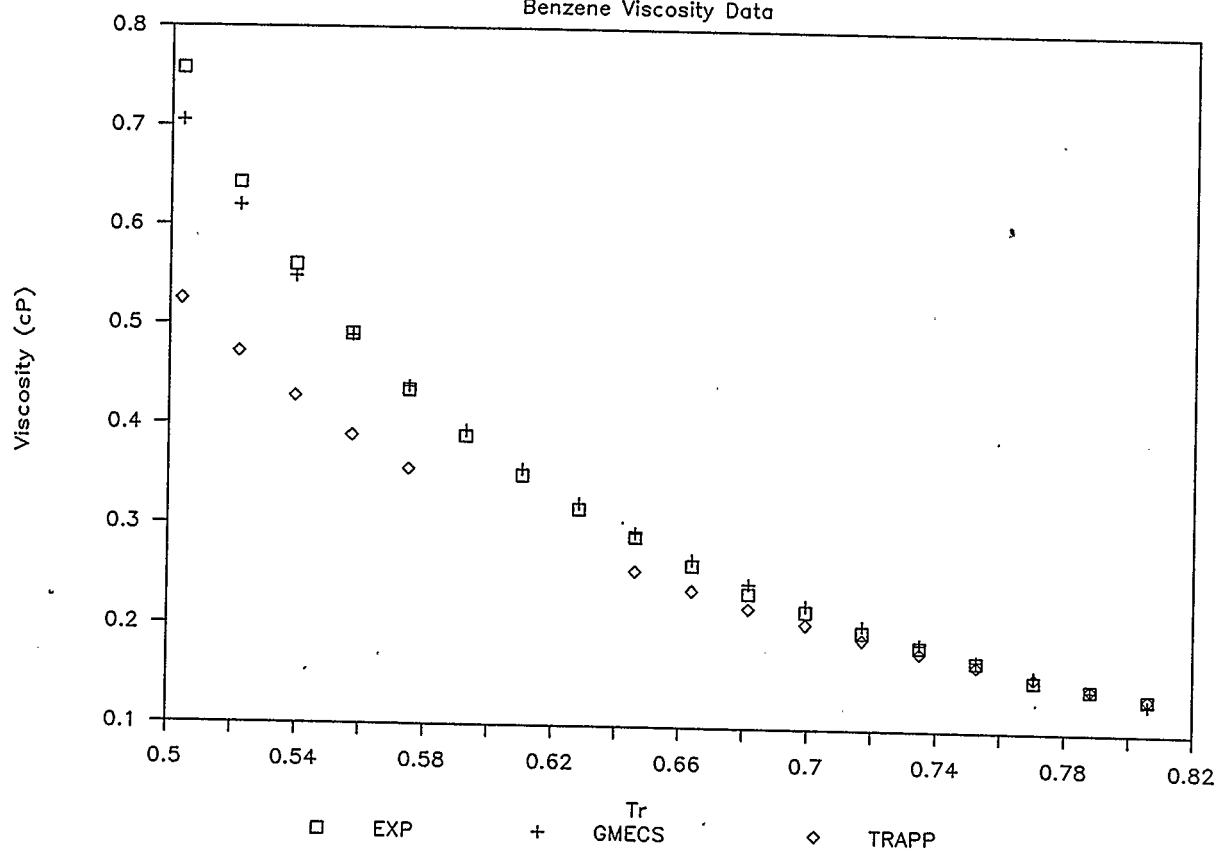


Table A-38
Toluene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4278	1.0700	1.0779	
101.325	-10.00	0.4447	0.9010	0.9246	0.8568
101.325	0.00	0.4616	0.7710	0.8024	0.7517
101.325	10.00	0.4785	0.6678	0.7033	0.6653
101.325	20.00	0.4954	0.5848	0.6215	0.5932
101.325	30.00	0.5123	0.5187	0.5532	0.5324
101.325	40.00	0.5292	0.4636	0.4954	0.4807
101.325	50.00	0.5461	0.4176	0.4460	0.4362
101.325	60.00	0.5629	0.3790	0.4033	0.3975
101.325	70.00	0.5799	0.3450	0.3661	0.3638
101.325	80.00	0.5967	0.3160	0.3334	
101.325	90.00	0.6136	0.2900	0.3045	
101.325	100.00	0.6305	0.2680	0.2787	
350.00	120.00	0.6643	0.2260	0.2356	0.2445
500.00	140.00	0.6981	0.1990	0.1998	0.2118
700.00	160.00	0.7319	0.1720	0.1698	0.1844
900.00	180.00	0.7657	0.1520	0.1439	0.1611

Figure A-38

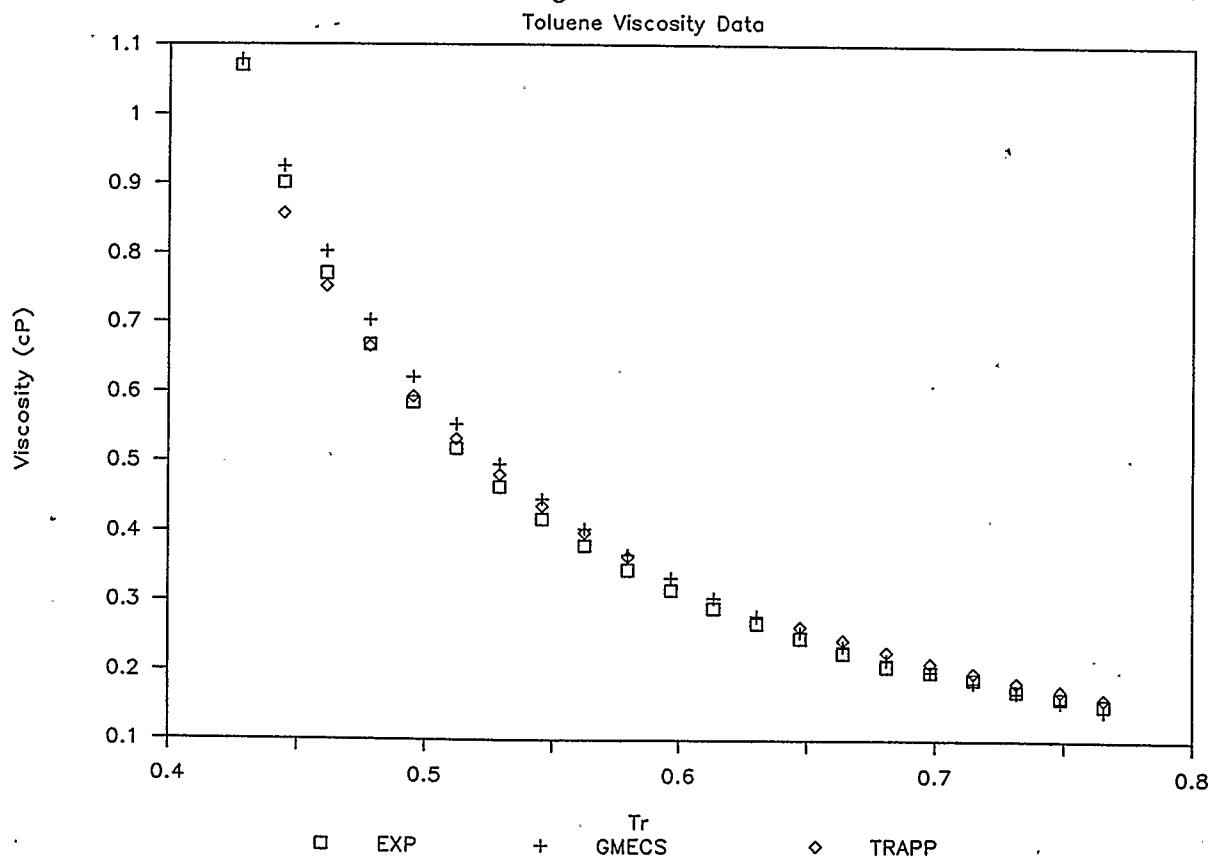


Table A-39
Ethylbenzene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.4102	1.2400	1.2138	
101.325	-10.00	0.4264	1.0420	1.0350	1.0967
101.325	0.00	0.4426	0.8920	0.8938	0.9512
101.325	10.00	0.4587	0.7728	0.7802	0.8333
101.325	20.00	0.4749	0.6763	0.6872	0.7364
101.325	30.00	0.4911	0.5985	0.6100	0.6557
101.325	40.00	0.5074	0.5338	0.5451	0.5878
101.325	50.00	0.5236	0.4800	0.4899	0.5300
101.325	60.00	0.5398	0.4350	0.4425	0.4804
101.325	70.00	0.5559	0.3960	0.4014	0.4374
101.325	80.00	0.5722	0.3630	0.3655	0.3999
101.325	90.00	0.5884	0.3330	0.3338	0.3670
101.325	100.00	0.6046	0.3070	0.3057	
101.325	110.00	0.6207	0.2850	0.2806	
101.325	120.00	0.6369	0.2640	0.2580	
101.325	130.00	0.6532	0.2460	0.2376	
101.325	140.00	0.6694	0.2300	0.2191	

Figure A-39
Ethylbenzene Viscosity Data

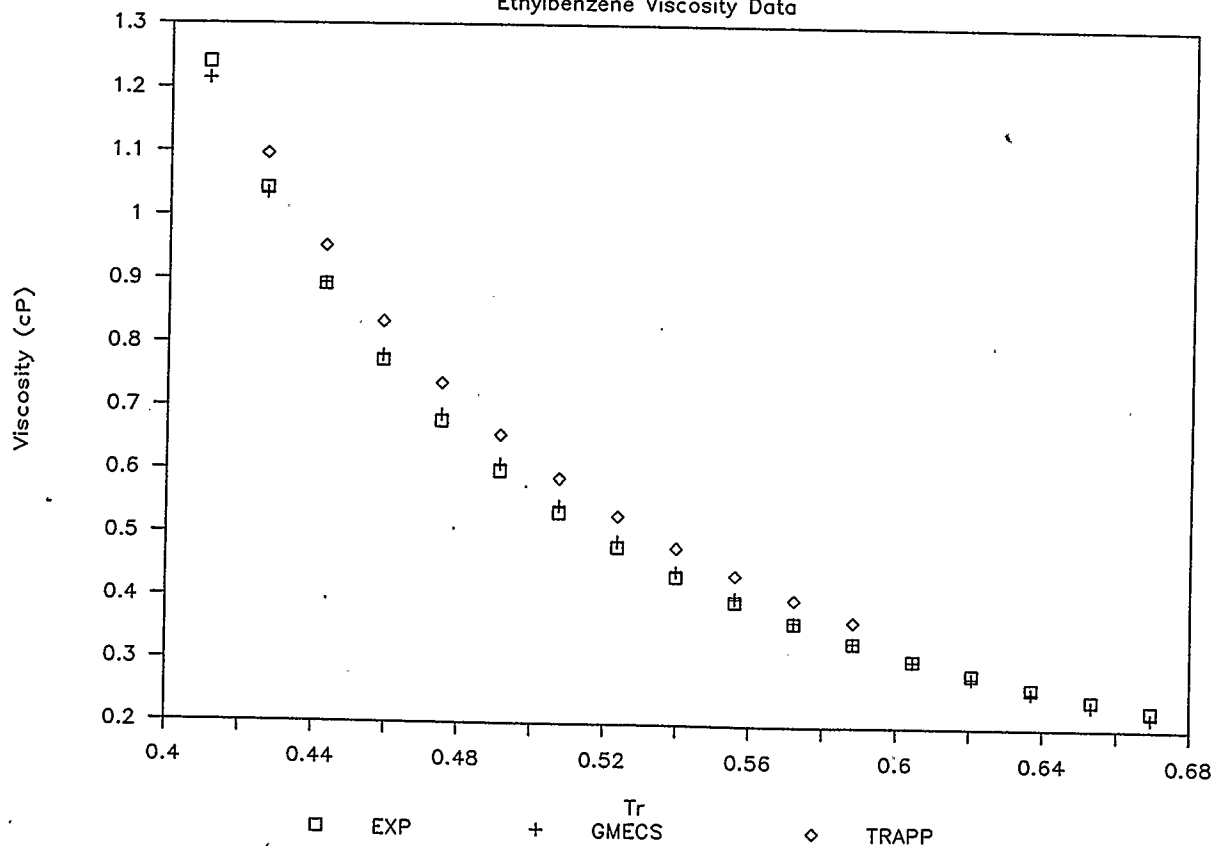


Table A-40
O-Xylene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	0.00	0.4334	1.1050	0.9767	1.0766
101.325	10.00	0.4492	0.9360	0.8495	0.9395
101.325	20.00	0.4651	0.8070	0.7461	0.8273
101.325	30.00	0.4809	0.7060	0.6606	0.7345
101.325	40.00	0.4968	0.6230	0.5891	0.6566
101.325	50.00	0.5127	0.5550	0.5285	0.5907
101.325	60.00	0.5286	0.5000	0.4766	0.5343
101.325	70.00	0.5444	0.4520	0.4317	0.4856
101.325	80.00	0.5603	0.4110	0.3926	0.4432
101.325	90.00	0.5762	0.3750	0.3583	0.4061
101.325	100.00	0.5920	0.3440	0.3279	0.3734
101.325	110.00	0.6079	0.3170	0.3008	
101.325	120.00	0.6237	0.2930	0.2765	
101.325	130.00	0.6396	0.2710	0.2546	
101.325	140.00	0.6555	0.2530	0.2348	

Figure A-40

O-Xylene Viscosity Data

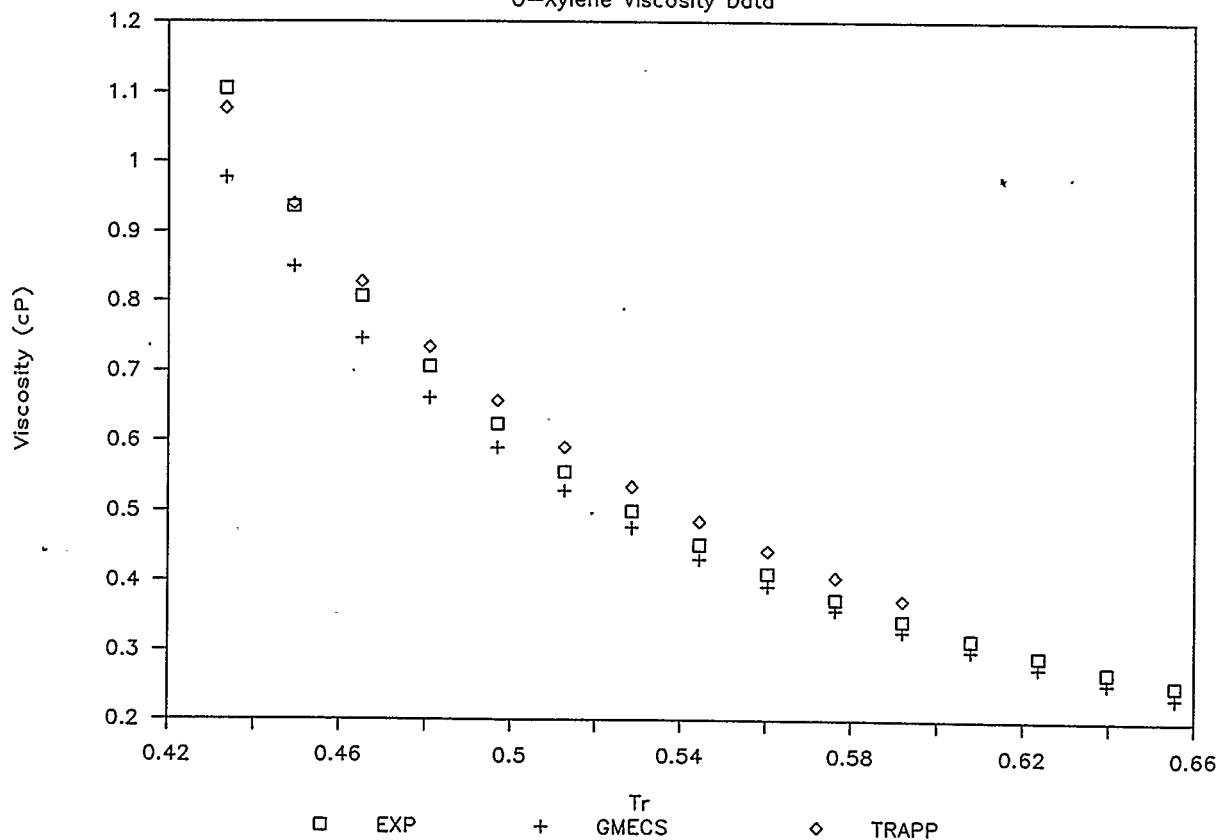


Table A-41
M-Xylene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	0.00	0.4427	0.8060	0.9101	0.9968
101.325	10.00	0.4589	0.7000	0.7936	0.8704
101.325	20.00	0.4751	0.6150	0.6984	0.7669
101.325	30.00	0.4913	0.5470	0.6196	0.6811
101.325	40.00	0.5075	0.4910	0.5533	0.6091
101.325	50.00	0.5237	0.4440	0.4970	0.5480
101.325	60.00	0.5399	0.4040	0.4487	0.4957
101.325	70.00	0.5561	0.3690	0.4069	0.4505
101.325	80.00	0.5723	0.3390	0.3703	0.4112
101.325	90.00	0.5885	0.3130	0.3381	0.3767
101.325	100.00	0.6047	0.2890	0.3096	
101.325	110.00	0.6209	0.2680	0.2841	
101.325	120.00	0.6371	0.2490	0.2612	
101.325	130.00	0.6533	0.2320	0.2406	
101.325	140.00	0.6696	0.2170	0.2218	

Figure A-41

M-Xylene Viscosity Data

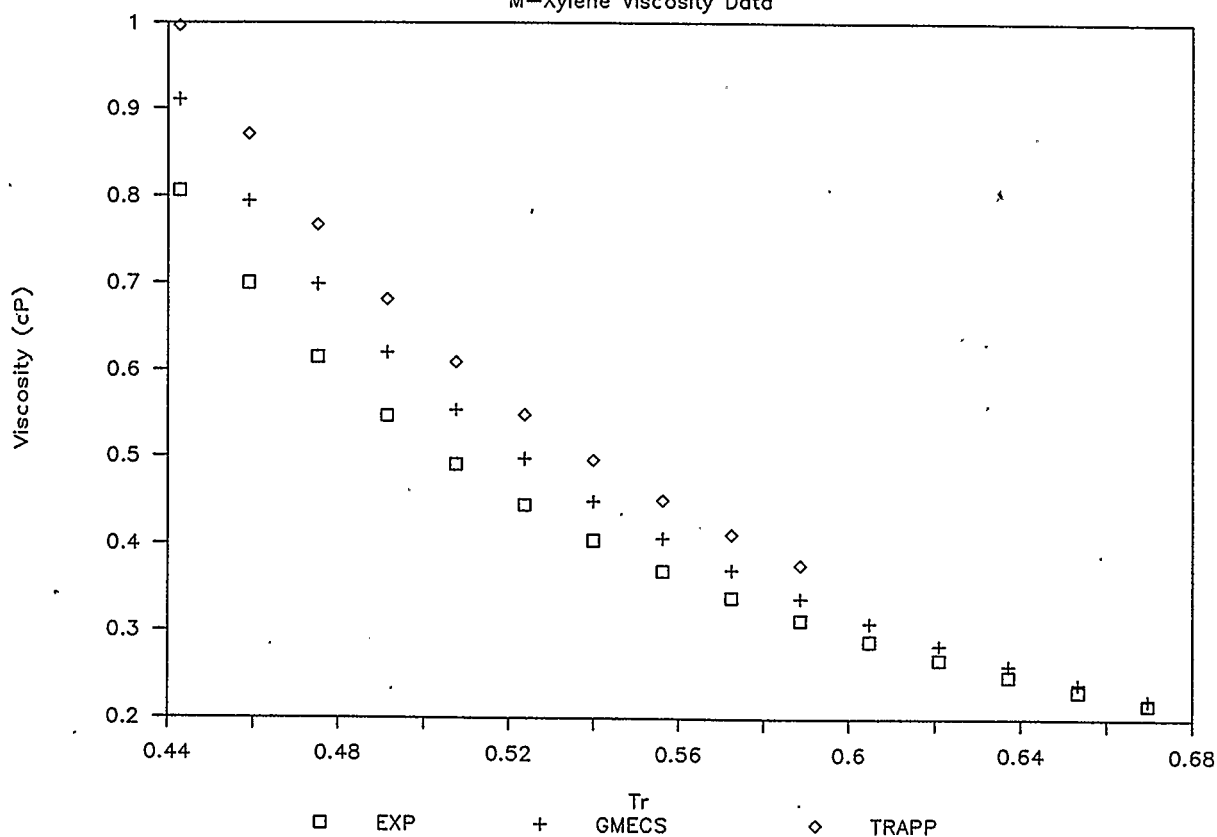


Table A-42
P-Xylene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	20.00	0.4757	0.6420	0.6903	0.7530
101.325	30.00	0.4916	0.5680	0.6125	0.6691
101.325	40.00	0.5082	0.5060	0.5471	0.5987
101.325	50.00	0.5244	0.4560	0.4915	0.5389
101.325	60.00	0.5407	0.4140	0.4438	0.4877
101.325	70.00	0.5569	0.3760	0.4025	0.4434
101.325	80.00	0.5731	0.3450	0.3664	0.4049
101.325	90.00	0.5893	0.3170	0.3345	0.3710
101.325	100.00	0.6056	0.2920	0.3063	
101.325	110.00	0.6218	0.2690	0.2811	
101.325	120.00	0.6380	0.2490	0.2585	
101.325	130.00	0.6542	0.2320	0.2380	
101.325	140.00	0.6705	0.2160	0.2195	

Figure A-42

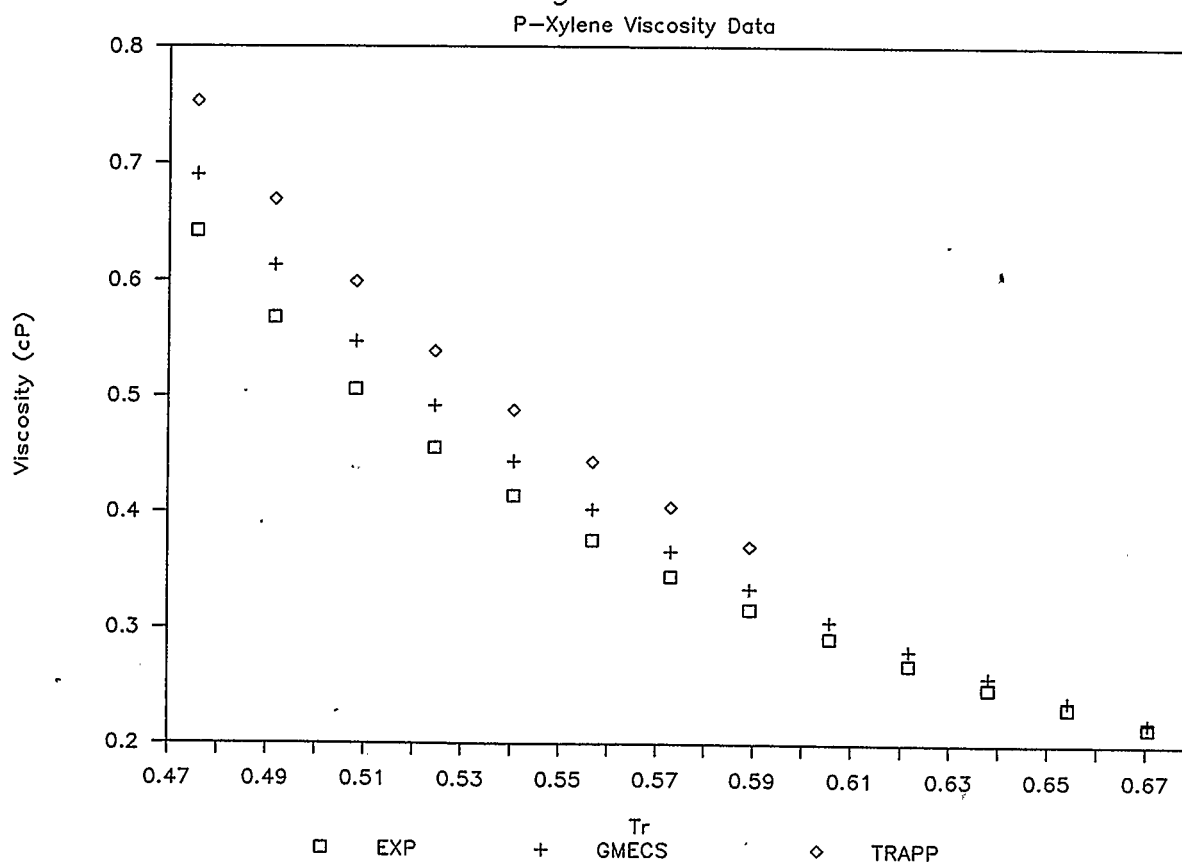


Table A-43

N-Propylbenzene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.3966	1.7100	1.5140	
101.325	-10.00	0.4123	1.4120	1.2702	
101.325	0.00	0.4279	1.1780	1.0818	1.2070
101.325	10.00	0.4436	0.9966	0.9332	1.0459
101.325	20.00	0.4593	0.8545	0.8137	0.9153
101.325	30.00	0.4749	0.7444	0.7160	0.8080
101.325	40.00	0.4906	0.6550	0.6350	0.7187
101.325	50.00	0.5063	0.5825	0.5670	0.6436
101.325	60.00	0.5219	0.5220	0.5092	0.5798
101.325	70.00	0.5376	0.4720	0.4597	0.5250
101.325	80.00	0.5532	0.4290	0.4168	0.4776
101.325	90.00	0.5689	0.3910	0.3793	0.4363
101.325	100.00	0.5846	0.3590	0.3463	0.4000
101.325	110.00	0.6002	0.3300	0.3171	0.3679
101.325	120.00	0.6159	0.3050	0.2910	
101.325	130.00	0.6316	0.2830	0.2677	
101.325	140.00	0.6472	0.2600	0.2466	

Figure A-43

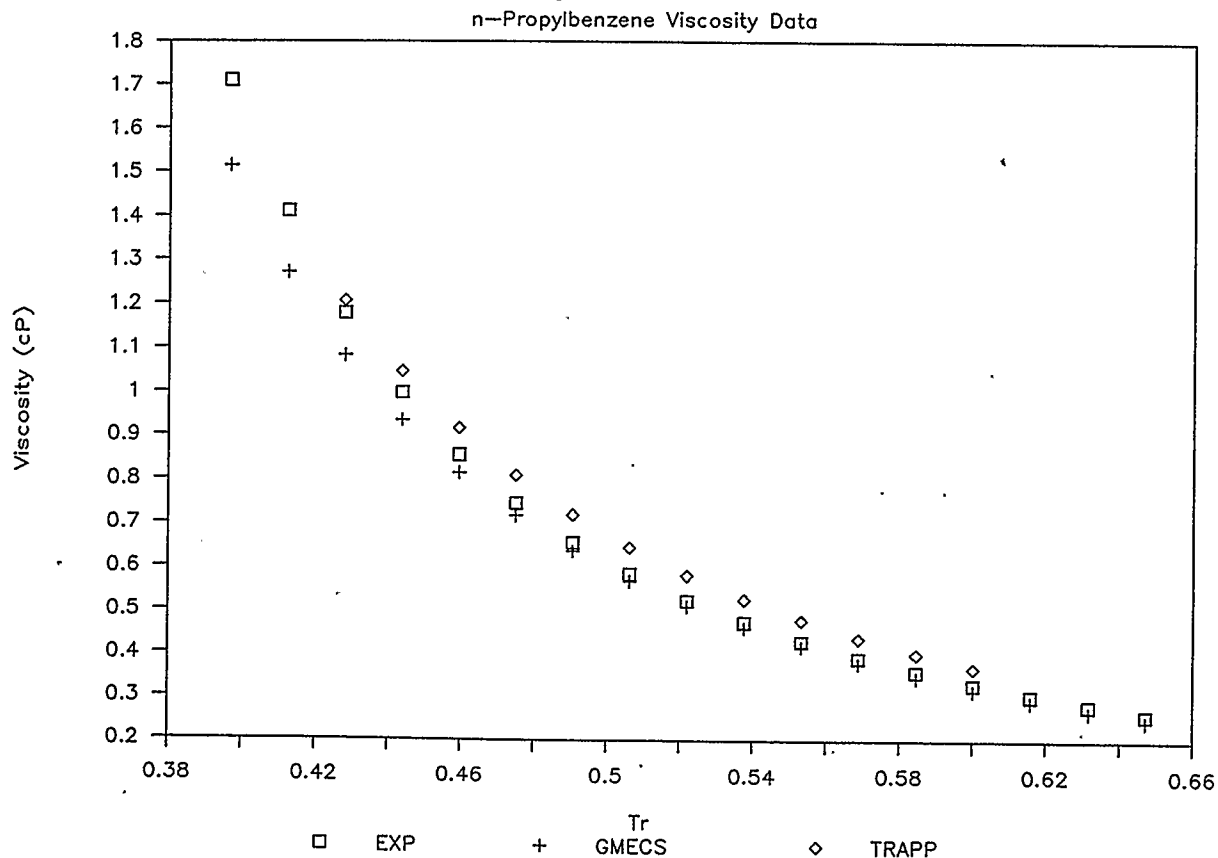


Table A-44
Isopropylbenzene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	0.00	0.4196	1.0730	1.0391	1.0650
101.325	10.00	0.4345	0.9140	0.8996	0.9275
101.325	20.00	0.4503	0.7890	0.7869	0.8154
101.325	30.00	0.4657	0.6910	0.6943	0.7228
101.325	40.00	0.4810	0.6100	0.6173	0.6454
101.325	50.00	0.4964	0.5430	0.5524	0.5800
101.325	60.00	0.5118	0.4890	0.4970	0.5242

Figure A-44

Isopropylbenzene Viscosity Data

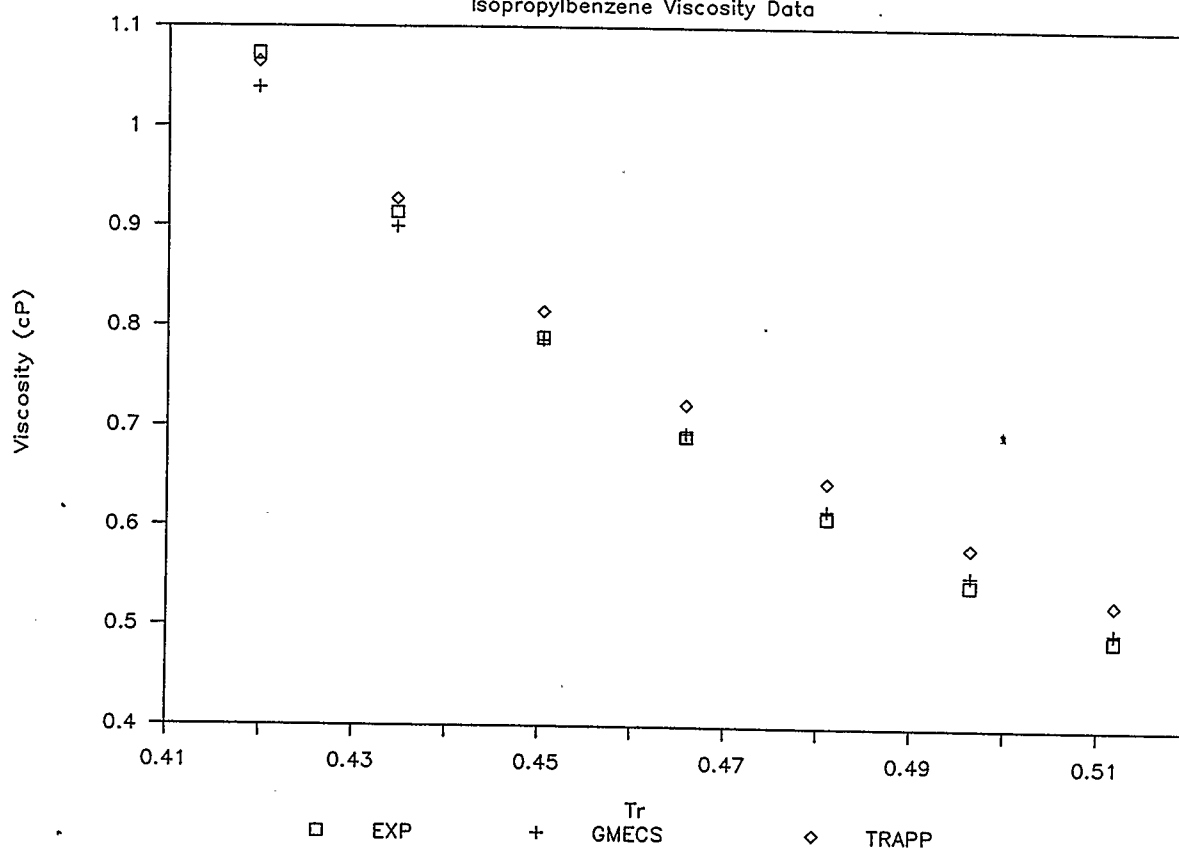


Table A-45
N-Butylbenzene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	-20.00	0.3833	2.2200	2.2567	2.2579
101.325	-10.00	0.3984	1.7850	1.8349	1.8751
101.325	0.00	0.4135	1.4620	1.5218	1.5814
101.325	10.00	0.4287	1.2160	1.2831	1.3515
101.325	20.00	0.4438	1.0320	1.0970	1.1685
101.325	30.00	0.4589	0.8910	0.9490	1.0203
101.325	40.00	0.4741	0.7790	0.8293	0.8988
101.325	50.00	0.4893	0.6820	0.7310	0.7979
101.325	60.00	0.5044	0.6120	0.6491	0.7132
101.325	70.00	0.5195	0.5480	0.5802	0.6413
101.325	80.00	0.5347	0.4960	0.5214	0.5797
101.325	90.00	0.5498	0.4490	0.4709	0.5266
101.325	100.00	0.5649	0.4100	0.4270	0.4804
101.325	110.00	0.5801	0.3800	0.3887	0.4399
101.325	120.00	0.5952	0.3500	0.3549	0.4041
101.325	130.00	0.6104	0.3200	0.3249	0.3724
101.325	140.00	0.6255	0.3000	0.2982	

Figure A-45
n-Butylbenzene Viscosity Data

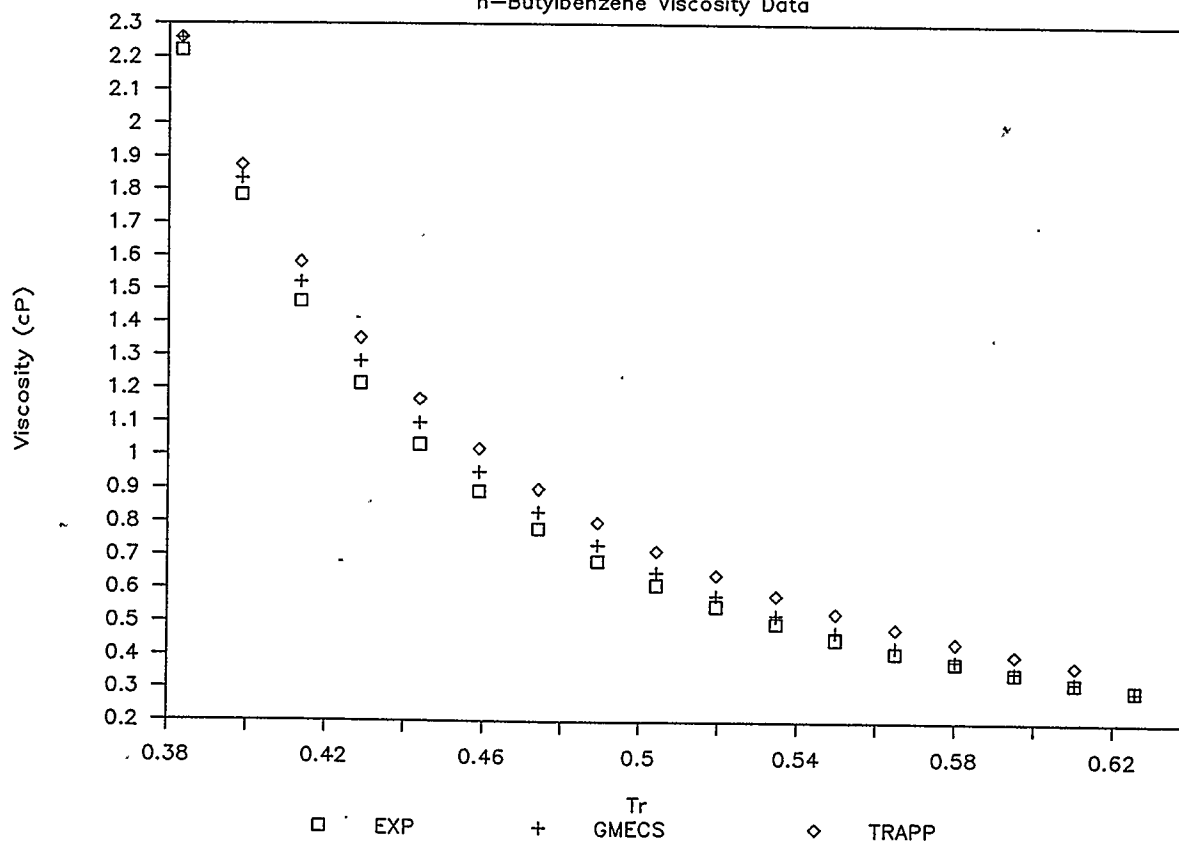
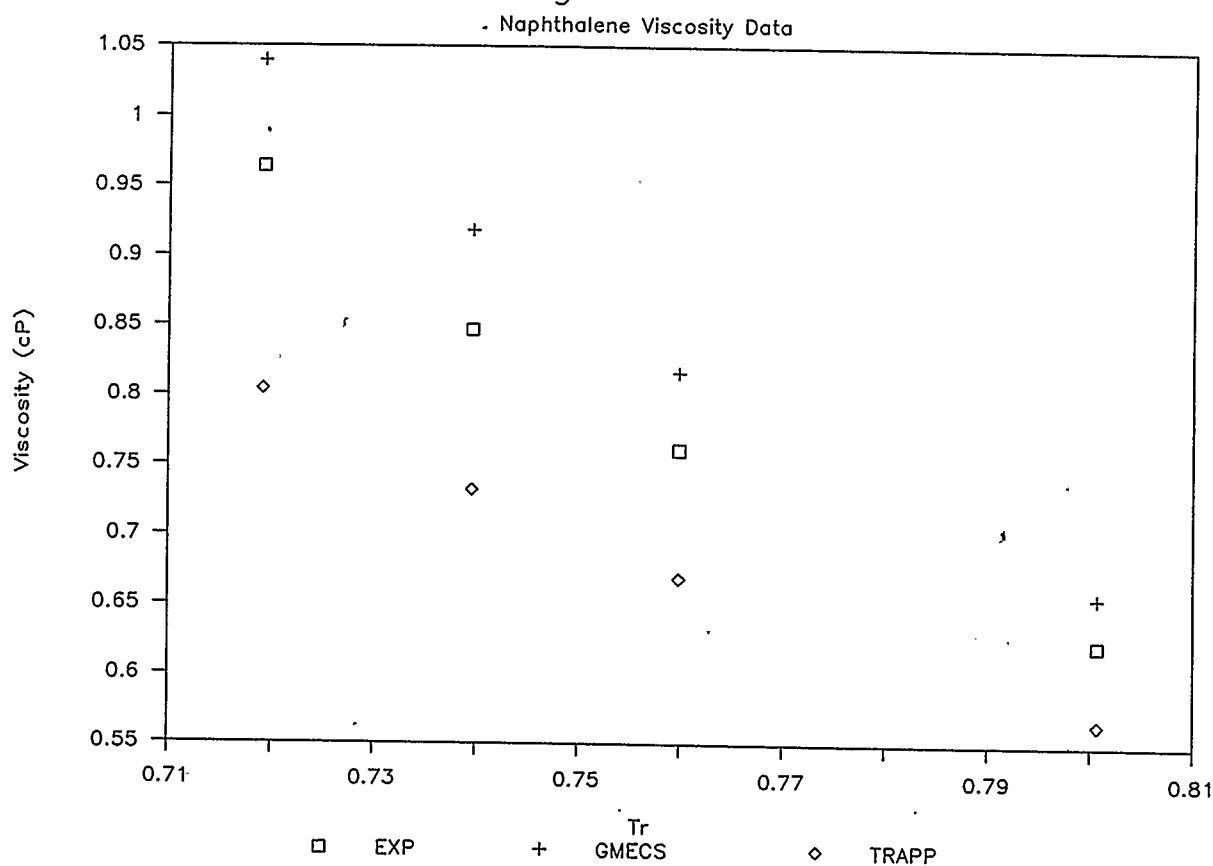


Table A-46
Naphthalene Viscosity Data

P(kPa)	T(C)	Tr	Viscosity (cP)		
			Exp.	GMECS	TRAPP
101.325	80.00	0.7192	0.9640	1.0397	0.8041
101.325	90.00	0.7396	0.8470	0.9183	0.7319
101.325	100.00	0.7599	0.7610	0.8167	0.6692
101.325	120.00	0.8007	0.6230	0.6571	0.5660

Figure A-46



APPENDIX B

Properties of Database Components

Compound	Pc (atm.)	Vc (cm ³ /gmol)	Tc (K)	OMEGA	M	Tb (K)
Paraffins						
CH ₄	45.387	97.752	190.56	0.0113	16.043	111.6
C ₂ H ₆	48.077	147.06	305.33	0.1004	30.070	184.6
C ₃ H ₈	41.914	201.61	369.82	0.1542	44.097	231.1
N-C ₄ H ₁₀	37.465	256.41	425.16	0.2004	58.124	272.2
I-C ₄ H ₁₀	36.003	263.00	408.15	0.1830	58.124	261.4
N-C ₅ H ₁₂	33.319	313.60	469.75	0.2511	72.151	309.2
I-C ₅ H ₁₂	33.368	306.00	460.43	0.2270	72.151	301.0
N-C ₆ H ₁₄	29.884	373.22	507.89	0.2978	86.178	341.9
N-C ₇ H ₁₆	26.997	431.97	540.14	0.3499	100.206	371.6
N-C ₈ H ₁₈	24.650	490.00	568.82	0.3995	114.232	398.8
C ₉ H ₂₀	22.576	548.90	594.56	0.4451	128.259	424.0
C ₁₀ H ₂₂	20.693	607.53	617.55	0.4885	142.287	447.3
C ₁₁ H ₂₄	19.130	665.00	638.74	0.5301	156.314	469.1
C ₁₂ H ₂₆	17.828	719.70	658.25	0.5708	170.341	489.5
C ₁₃ H ₂₈	16.610	775.20	676.15	0.6096	184.368	508.6
C ₁₄ H ₃₀	15.525	827.13	692.95	0.6442	198.395	526.7
C ₁₅ H ₃₂	14.459	880.28	706.75	0.6918	212.422	543.8
C ₁₆ H ₃₄	13.576	930.23	720.55	0.7311	226.449	560.0
C ₁₇ H ₃₆	12.748	977.00	733.35	0.7623	240.476	575.2
C ₁₈ H ₃₈	11.843	1030.00	748.20	0.7900	254.504	589.5
C ₁₉ H ₄₀	11.000	1085.00	756.00	0.8270	268.529	603.1
C ₂₀ H ₄₂	10.955	1140.00	767.00	0.9070	282.566	617.0
Olefins						
C ₂ H ₄	49.700	129.00	282.40	0.0850	28.054	169.3
C ₃ H ₆	45.408	181.00	364.85	0.1440	42.081	225.5
1-C ₄ H ₈	39.700	240.00	419.60	0.1870	56.108	266.9
1-C ₅ H ₁₀	40.000	300.00	464.70	0.2450	70.135	303.1

Compound	Pc (atm.)	Vc (cm ³ /gmol)	Tc (K)	OMEGA	M	Tb (K)
1-C ₆ H ₁₂	31.300	350.00	504.00	0.2850	84.162	336.6
Cyclopentanes						
C ₅ H ₁₀	44.491	260.00	511.70	0.1960	70.135	322.4
C ₆ H ₁₂	37.345	319.90	532.73	0.2310	84.162	345.0
C ₇ H ₁₄	33.426	375.00	569.50	0.2710	98.189	376.6
C ₈ H ₁₆	29.805	427.00	596.20	0.3350	112.216	404.1
Cyclohexanes						
C ₆ H ₁₂	40.168	308.00	553.50	0.2120	84.162	353.8
C ₇ H ₁₄	34.256	368.00	572.20	0.2360	98.189	374.1
C ₈ H ₁₆	29.900	450.00	609.00	0.2430	112.216	404.9
C ₉ H ₁₈	26.746	472.00	639.00	0.2580	126.243	432.4
C ₁₀ H ₂₀	31.088	527.00	667.00	0.3620	140.260	454.1
Aromatics						
C ₆ H ₆	48.340	259.00	562.16	0.2120	78.110	353.2
C ₇ H ₈	40.503	316.00	591.79	0.2630	92.140	383.8
C ₈ H ₁₀	35.529	374.00	617.20	0.3020	106.170	409.3
O-C ₈ H ₁₀	36.812	369.00	630.30	0.3100	106.170	417.6
M-C ₈ H ₁₀	34.888	376.00	617.05	0.3250	106.170	412.3
P-C ₈ H ₁₀	34.651	379.00	616.20	0.3210	106.170	411.5
N-C ₉ H ₁₂	31.581	440.00	638.32	0.3440	120.195	432.4
I-C ₉ H ₁₂	30.002	429.00	651.00	0.3260	120.195	425.6
N-C ₁₀ H ₁₄	28.522	497.00	660.50	0.3930	134.222	456.5
C ₁₀ H ₈	39.970	413.00	748.40	0.2690	128.174	491.1

APPENDIX C

Reference Fluid Viscosity and Density Constants

Reference Fluid Viscosity Constants

i	a_i	b_i	c_i
1	-0.113610292E+02	0.00	-3.032813828E+00
2	0.799163527E+03	0.00	1.691888009E+01
3	0.183214031E+02	1.12	-3.718936492E+01
4	-0.143272346E+05	359.00	4.128886186E+01
5	0.157156242E+00		-2.461592114E+01
6	0.190927109E+03		8.948843096E+00
7	0.317861154E+05		-1.873924504E+00
8			2.096610139E-01
9			-9.657043707E-03
10			8.020651288E+00

Reference Fluid Density (COSTALD) Constants

For propane: $\omega_{\text{SRK}} = 0.1532$ $V^* = 0.2001$

Saturated Volume Constants

$a = -1.52816$
 $b = 1.43907$
 $c = -0.81446$
 $d = 0.190454$
 $e = -0.296123$
 $f = 0.386914$
 $g = -0.0427258$
 $h = -0.0480645$

Compressed Liquid Constants

$$a = -9.070217$$

$$b = 62.45326$$

$$d = -135.1102$$

$$f = 4.79594$$

$$g = 0.250047$$

$$h = 1.14188$$

$$j = 0.0861488$$

$$k = 0.0344483$$