

**STUDY ON THERMODYNAMIC  
PROPERTIES OF MTBE / ALCOHOL BINARY  
MIXTURES USING NONLINEAR MODELS  
AND MOLECULAR INERACTONS USING  
SPECTROSCOPIC APPROACH**

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### **SUPERVISOR'S DECLARATION**

We hereby declare that we have checked this thesis and in our opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Master of Engineering in Chemical Engineering

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**THANUSHA A/P THANIHAIK KUMAAR**

Thesis submitted in fulfillment of the requirements  
for the award of the degree of  
Master of Engineering (Chemical)

Faculty of Chemical & Natural Resources Engineering

UNIVERSITI MALAYSIA PAHANG

APRIL 2017

## **DEDICATION**

I specially dedicate this dissertation  
To my beloved parents Thanihaik Kumaar and Suganthy,  
& my supervisor Dr. Ramesh Kanthasamy  
for their continuous support and sacrifice throughout my studies and life

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## LIST OF SYMBOLS

%	Percentage
-	Subtract
+	Add
×	Multiply
=	Equal to
<	Less than
>	More than
$\leq$	Less than or equal to
$\geq$	More than or equal to
$^{\circ}\text{C}$	Degree Celcius
s	second
atm	Atmospheric Pressure
cm	Centimetre
$\text{cm}^{-1}$	Reciprocal centimetre
ml	Millilitre
g	Gram
$\text{g}/\text{cm}^3$	Gram per cubic centimetre
$\text{g}/\text{mol}$	Gram per mol
$\text{m}^2/\text{s}$	Square metre per second
mPa.s	Megapascal second
$\text{cm}^3/\text{mol}$	Cubic centimetre per mol
$\varphi$	Volume fraction
$x$	Mole fraction
$\omega$	Mass fraction
$\sigma$	Standard deviation
$\rho$	Density
$\eta$	Dynamic viscosity
$\nu$	Kinematic viscosity
$E^\nu$	Activation energy
R	Universal Gas Constant
N	Avagrado's number
h	Plank's constant
V	Molar volume
M	Molecular mass
$\text{V}^E$	Excess molar volume

$\Delta\eta$	Viscosity deviation
$\Delta G^*$	Free energy of activation
$A_j$	Model constants
$j$	Number of coefficients
$G_{12}$	Grunberg-Nissan constant
$Z_{12}, Z_{21}$	McAllister interaction parameters
$\delta$	Chemical shift

## **LIST OF ABBREVIATIONS**

<sup>1</sup> H-NMR	Proton Nuclear Magnetic Resonance
ATR-FTIR	Attenuated Total Reflectance-Fourier Transform Infrared
MTBE	Methyl-tert butyl ether
COP21/CMP11	21 <sup>st</sup> session of the Conference of the Parties and the 11 <sup>th</sup> meeting of the Parties to the Kyoto Protocol
MW	Molecular Weight

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## **ABSTRAK**

Sejak kebelakangan ini, aditif beroksigenat bahan api telah menarik perhatian disebabkan oleh peningkatan kebimbangan alam sekitar dan permintaan bahan api. Campuran perduaan bahan api beroksigenat meningkatkan prestasi enjin berbanding oksigenat bahan api tulen. Oleh itu, campuran bahan api ini dijangka dapat mengurangkan pelepasan gas daripada kenderaan. Formulasi baru campuran ini akan menjadi masalah dalam hal menentukan gabungan sesuai untuk dicampur dalam petrol atau semasa pengiraan reka bentu proses jika sifat termofizikal mereka tidak diketahui. Selain itu, ianya juga penting untuk mengenal pasti model ramalan bukan linear untuk sifat-sifat termofizikal campuran ini supaya dapat mengurangkan kesukaran dalam kerja kerja ujikaji pada masa depan dan menyediakan cara yang lebih cepat untuk meramalkan sifat-sifat termodifizikal campuran ini. Di samping itu, pengetahuan tentang kewujudan interaksi molekul dalam campuran perduaan ini juga penting untuk menentukan kestabilan mereka apabila dicampur dengan petrol.

Campuran perduaan MTBE dengan etanol, 1-propanol dan 1-butanol dipertimbangkan dalam kajian ini oleh kerana keupayaan meningkatkan oktana dalam bahan api. Ketumpatan dan kelikatan campuran MTBE dengan etanol, 1-propanol dan 1-butanol pada suhu 30 °C, 35 °C, 40 °C and 45 °C telah diukur pada julat keseluruhan komposisi. Data ketumpatan telah dikorelasi dengan model Jouyban-Acree manakala data kelikatan telah dikorelasi dengan model Grunberg-Nissan, McAllister, Ausländer and Jouyban-Acree. Lebihan isipadu molar dan deviasi kelikatan telah dikira dari data ujikaji dan dikorelasi dengan model polinomial Redlich-Kister. Perubahan yang diperhatikan dalam sifat-sifat lebihan termofizikal dari segi komposisi dan suhu dibincangkan dari segi interaksi molekul disebabkan oleh kesan fizikal dan kimia antara molekul yang berbeza. Analisis spektroskopi ATR-FTIR dan  $^1\text{H-NMR}$  telah dijalankan sebagai bukti selanjutnya untuk mengkaji interaksi antara molekul dalam campuran. Kewujudan interaksi telah disahkan dengan perubahan dalam anjakan band dan perbezaan puncak intensiti komponen tulen dan campuran perduaan.

Daripada kajian ini, model Jouyban-Acree telah dikenal pasti sebagai model yang tepat untuk mengukur data ketumpatan ketiga-tiga campuran perduaan ini dengan mempunyai sisihan piawai dalam julat 0.00028 ke 0.00066, manakala model Ausländer telah dikenal pasti memberi ketepatan yang baik untuk mengukur data kelikatan ketiga-tiga campuran perduaan ini. Kewujudan interaksi kuat antara molekul adalah berkemungkinan seperti yang diperhatikan dari sifat-sifat berlebihan dan keputusan dari analisis spektroskopi ATR-FTIR dan  $^1\text{H-NMR}$ . Dua jenis interaksi berkemungkinan yang diperhatikan dalam campuran perduaan ini ialah pembentukan ikatan hidrogen dan geometri gegasan antara komponen dalam campuran perduaan ini.

## ABSTRACT

Over the years, fuel additive oxygenates have attracted a great interest due to the increasing environmental concern and fuel demand. Binary fuel oxygenate mixtures are believed to increase the performance of engine compared to pure fuel oxygenates. Thus, they are expected to reduce emission from vehicles. The problem that lies in obtaining the new formulation of binary fuel oxygenate mixtures is lack of data on their complete thermodynamic properties. Problems may arise in determining proper fuel blend or process design calculations when the thermodynamic properties are not known. There is also lacking in study on nonlinear models for the prediction of density and viscosity of the mixtures. In addition, it is also essential to know about the presence of molecular interaction of these binary mixtures to determine their stability when blended with gasoline.

The binary mixtures of MTBE with ethanol, 1-propanol and 1-butanol are considered in this study due to their octane enhancing ability. Density and viscosity of MTBE with ethanol, 1-propanol and 1-butanol mixtures at temperatures 30 °C, 35 °C, 40 °C and 45 °C have been measured at selected range of composition. The density data are correlated with Jouyban-Acree model, whereas the viscosity data are correlated with Grunberg-Nissan, McAllister, Ausländer and Jouyban-Acree model. The model parameters are computed using least-square method. The excess molar volume and viscosity deviation are calculated from the experimental data and correlated with Redlich-Kister model. The observed variation in the excess functions in terms of composition and temperature, are discussed in terms of molecular interaction due to physical and chemical effect between the unlike molecules. Attenuated total reflectance-fourier transform infrared (ATR-FTIR) and proton nuclear magnetic resonance ( $^1\text{H-NMR}$ ) spectroscopy analysis was also done to provide evidence on the molecular interactions taking place in the mixtures. The presence of interaction was confirmed with change in band shift and difference in peak intensity of the binary mixtures and pure components.

The results concluded that Jouyban-Acree model was a precise model for density measurement of the three mixtures having standard deviation in the range of 0.00028 to 0.00066, whereas Ausländer model has given good accuracy for viscosity measurement. ATR-FTIR and  $^1\text{H-NMR}$  analysis and excess properties of the binary mixtures shows that there may be strong interaction present between the components in the binary mixtures. The two possible interactions observed in the binary mixtures were hydrogen bond formation and geometrical fitting between the components in the binary mixtures.

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