

**Phase Equilibrium Studies for the Development of Fuel
Systems and LPG Fuel Mixture Using Regular Solution**

Theory

By

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NOMENCLATURE

| Symbol | Description | Unit |
|----------|---|--------|
| T_b | Temperature of the component | (°C) |
| T_c | Critical temperature of the component | (°C) |
| P_c | Critical pressure of the component | (MPa) |
| P_i | Pressure of the component | (MPa) |
| Y_A | Mole fraction of component A in gas | |
| X_A | Mole fraction of component A in liquid | |
| H | Henry's Constant | |
| a_{JK} | Group interaction parameter | |
| Q^E | Excess Gibbs energy | J/gmol |
| N_i | Number of moles of species | |
| q_i | Area parameter of component i | |
| r_i | Volume parameter of component i | |
| Q_k | Area parameter, contribution of molecular group | |
| R_k | Volume parameter, contribution of molecular group | |

| | |
|-----------|---------------------------------------|
| R_v | Relative volatility |
| Z | Coordination number |
| w_k | Group mole fraction |
| D_{RF} | Detector response factors |
| $K_{A,B}$ | Capacity factors of component A and B |
| Q | Gibbs function |
| K | Vapor-liquid distribution |

Greek Symbols

| | |
|----------|-----------------------------|
| γ | Activity coefficients |
| ξ_k | Group surface area fraction |
| α | Selectivity of a component |
| θ | Area fraction of component |

ABBREVIATIONS

| | |
|------|-------------------------------------|
| AAD | Average Absolute deviations |
| CCS | Chemical Component System |
| DDB | Dortmund Data Bank |
| EOS | Equation of State |
| GC | Gas Chromatography |
| GCM | Group Contribution Method |
| GLC | Gas Liquid Chromatography |
| HMC | Heavy Molecular Components |
| HPLC | High Pressure Liquid Chromatography |
| LMC | Light Molecular Components |
| LNG | Liquid Natural Gas |
| LPG | Liquid Petroleum Gas |
| MHV | Mixing rule of Huron-Vidal |
| NRTL | Non-Random-To-Liquid |
| PVT | Pressure, Volume and Temperature |

| | |
|---------|--|
| SFC | Supercritical Fluid Chromatography |
| SFE | Supercritical Fluid Extraction |
| SRK | Soave-Redlich-Kwong |
| TCF | Trillion Cubic Feet |
| UNIFAC | Universal Functional Activity Coefficients |
| UNIQUAC | Universal Quasi Activity Coefficients |
| VLE | Vapor-Liquid Equilibrium |

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GLOSSARY

| English | Bahasa Malaysia |
|--------------------------------|---------------------------------------|
| Supercritical Fluid Extraction | Pengekstraken Bendalir Lampau Genting |
| Yield | Kadar hasil |
| Solubility | Keterlarutan |
| Density | Ketumpatan |
| Selectivity | Kemermilihan |
| Experimental Works | Kajian Ujikaji |
| Theoretical Works | Kajian Teoritical |
| Phase Equilibrium | Keseimbangan Fasa |
| Interaction Parameter | Parameter Interaksi |
| Group Contribution Method | Kedah Sumbangan Berkumpulan |
| Vapor-Liquid Equilibrium | Kieseimbangan Fasa Wap dan Cecair |
| Coordination Number | Nombor Koordinasi |
| Intermolecular Forces | Kekuasaan Antra Molekul |
| Mole Fraction | Mole Fraksi |

ABSTRAK

Tujuan kajian ini adalah untuk menilai tahap kelayakan proses keseimbangan kelarutan menggunakan propane superkritik. Sebuah model termodinamik berdasarkan pada kajian teori penyelesaian biasa untuk menilai kegiatan ekspresi pekali setiap tahap untuk campuran sebatian gas untuk meramal data kelarutan. Kegunaan persamaan diambil daripada teori penyelesaian termodinamik untuk mengumpul dan meramal kelarutan reksa yang dibincangkan dengan rujukan pasangan binari (propana / Heksana dan propana / dekana sistem). Hal ini boleh disimpulkan bahawa sesetengah pengiraan parameter diperlukan untuk pengiraan sebegini akan menjadi sukar jika heksana komponen terlarut atau berat atau dekana di LPG atau LNG yang peka terhadap suhu atau sebatian kompleks tentang yang dikenali untuk struktur formulanya. Satu prosedur alternatif kegiatan ekspresi pekali daripada teori penyelesaian biasa yang dikenali sebagai teori UNIFAC untuk setiap tahap. Perhitungan sepanjang garis-garis ini digambarkan dan dasar fizikal untuk melaksanakan kaedah ini adalah dalam keadaan yang relevan untuk dibincangkan. Pendekatan secara khusus teori UNIFAC telah dijumpai untuk berada pada ramalan yang baik untuk kajian system dan komposisi LNG LPG buat masa sekarang.

ABSTRACT

The objective of this work is the assessment of the feasibility studies of phase equilibria mutual solubility process utilizing subcritical propane. A thermodynamic model based on regular solution theory studies to evaluate activity coefficients expression to each the heavy compound such as (propane and hexane) and the solvent such as propane in order to predict mutual solubility data. The use of equations derived from thermodynamic of the regular solution theory for collecting and predicting mutual solubility discussed with reference to binary pairs (propane / hexane and propane / decane systems). It is concluded that the calculation of some of the parameters required for these calculation would be difficult if the solute or heavy component hexane or decane in LPG or LNG were sensitive to temperature or complex substance about which little was known apart for its structural formula. An alternative procedure is to apply activity coefficients expression of the regular solution theory from which is called Universal Functional Activity Coefficient theory (UNIFAC) to each phase. Calculation along these lines described and the physical basis for applying this method under the relevant condition discussed. The UNIFAC theory approach in particular has been found to be in good estimation for the present studies of these systems LNG and LPG composition.