



## THE STUDY OF MENTAL MODEL ON N-HEXANE-METHANOL BINARY SYSTEM (THE VALIDATION OF PHYSICAL CHEMISTRY PRACTICUM PROCEDURE)

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### ABSTRACT

N-hexane and methanol system is one example of a binary system that shows the solubility properties of reciprocity. This study aimed to assess the mental model of a n-hexane-methanol binary system. Interaction at the submicroscopic level between n-hexane and methanol molecules is described in the form of mental model. Penelitian ini menggunakan cloud point method untuk memperoleh data kesetimbangan cair-cair sistem n-heksana-metanol. This study used a cloud point method to obtain data on liquid-liquid equilibrium on the system of n-hexane-methanol. Research data showed the maximum critical temperature (above the consolute temperature) of this system was at 42.95 °C with  $X_{\text{methanol}} = 0.475$  ( $P = 715$  mmHg). Data from the laboratory observations was represented as a symbolic level in the form of the curve of correlation between mole fraction of methanol with temperature in a phase diagram system of n-hexane-methanol. The curve that was formed was asymmetric. It indicated that the solubility of n-hexane in methanol was relatively small compared to the solubility of methanol in n-hexane. Mental model of the binary system of n-hexane-methanol in four curve areas in the form of visualization of the interaction between n-hexane and methanol molecules through London force. In thermodynamics, each component had the same chemical potential in both phases at equilibrium state. This study results could have a contribution to form a mental model on the student as the prospective chemistry subject teachers.

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**Keywords:** n-hexane-methanol system; mental model, macroscopic level; submicroscopic level; symbolic level.

### INTRODUCTION

Physical chemistry is defined as the study of which is based on the principles of physics and mathematics terms that determines the properties and behavior of chemical systems. The physical chemistry could be investigated at the level of macroscopic, submicroscopic and symbolic. By studying the material of physical chemistry that refers to the phenomena observed (macroscopic), chemistry students can explain the phenomenon through submicroscopic explanation. The explanation at the submicroscopic level is strongly supports the symbolic explanation in the form of a derivative formula or a formula obtained from the

observed phenomena. In principle, the students need to associate the phenomenon of macroscopic, submicroscopic and symbolic in studying the material of physical chemistry. It is intended that the students as the teacher candidates must fully understand the chemistry, since they have to deliver it to their students in the future.

In order to achieve the goal of chemistry fully understanding, the scientists present the concept into three levels of representation to explain the chemical phenomena. First, the macroscopic level as the level that is consistent with the observation of concrete objects. At this level, the students observe the chemical phenomena in the experiment. Second, the submicroscopic level as an abstract level; however, it is related to a phe-

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nomenon that can be observed at the macroscopic level. This level is characterized by concepts, theories and principles used to explain what is observed at the macroscopic level, using things like the movement of electrons, molecules, atoms, or ions. Third, the symbolic level that is used to describe chemical reactions and macroscopic phenomena using chemical equations, mathematical equations, graphs, reaction mechanism, analogies, and certain models (Jansoon et al., 2009).

Chittleborough (2004) presented that the students' ability to understand and to decipher the chemistry representation reflects the level of their mental models. Greca and Moreira (in Wang & Barrow, 2010) described the mental models as an internal representation constructed by a person to understand or to give a rational explanation of a phenomenon of experience. Mental models are used to produce a simpler concept, providing support for the simulation and visualization, as well as providing explanations for scientific phenomena (Coll, 2009).

The results of research by Nyachwaya & Wood (2014) showed that most physical chemistry textbooks omit discussion of how to link the mathematical representations to the macroscopic level or submicroscopic level. The use of multiple representations to associate the macroscopic level with submicroscopic level and symbolic level is very limited, not more than 1% of the overall pictures in the textbook. It is also found in the laboratory component in the physical chemistry lecture. The lack of use of this multiple representations certainly impacts the formation of student mental models.

Phase equilibrium is one of the study materials in physical chemistry lecture. The results of the previous studies indicated that there has been a student misunderstanding about the concept of vapor pressure equilibrium, phase diagrams, phase changes, colligative properties and Rault's law (Azizoglu et al., 2006). Also, there have been the misinterpretation on the concept of evaporation and vapor pressure (Conpolat et al., 2006) and misconceptions on the concept of evaporation, condensation and vapor pressure (Gopal et al., 2004).

Binary system is one of the topics of phase equilibrium in the physical chemistry lecture that is studied by the students of chemistry teacher candidates. To date, the research on the topic of binary systems is only focus to examine the behavior of binary systems in the laboratory (Dai & Chao, 1985; Alessi et al, 1989). There are no studies which evaluating the binary system by linking the three levels of the chemical represen-

tation. System of n-hexane and methanol is one example of a binary system which shows the solubility properties of reciprocity as the focus of this study. The interaction that occurs in the system of n-hexane-methanol at a submicroscopic level is depicted in the form of mental models. This study aimed to assess the further mental model of the binary system of n-hexane-methanol. This study was intended to contribute the formation of a mental model of the student of chemistry teacher candidates.

## METHODS

This study was a validation of the binary system practicum procedure by using the cloud point method. The tools used in this study were test tubes, corks as the tube plug, beakers, hot plate with a magnetic stirrer, the stand and clamp, thermometers, measuring pipettes and the ball respirators. Materials used to support the system were n-hexane and methanol (Pro-Analysis Grade).

The temperature of the water bath used was set at  $\pm 55$  °C to prevent the fast evaporation process of methanol. Methanol in amount of 0.1 ml ( $\pm 2$  drops) was incorporated into 5 ml n-hexane in a test tube. When the obtained solution was not cloudy, the solution was then added back by 0.1 ml of methanol. But if the solution turned cloudy, the reaction tube was closed using the cork. The test tube was then heated along with its contents in the bath while stirring. The temperature of the mixture was recorded exactly when the mixture turned from cloudy to clear ( $T_1$ ). The test tube was removed from the water bath, and then it was allowed to stand while stirring until cool. The temperature of the mixture was also recorded at the time of cloudy was appearing ( $T_2$ ). Based on this data, the mean temperature (T) was calculated and was accounted. These steps were repeated for several times. Data obtained from the optimization of n-hexane and methanol system lab procedures was subsequently assessed descriptively by explaining in the submicroscopic and symbolic level.

## RESULTS AND DISCUSSION

The study was conducted at 715 mmHg air pressure. Table 1 represents the information about the physical and chemical properties of substances.

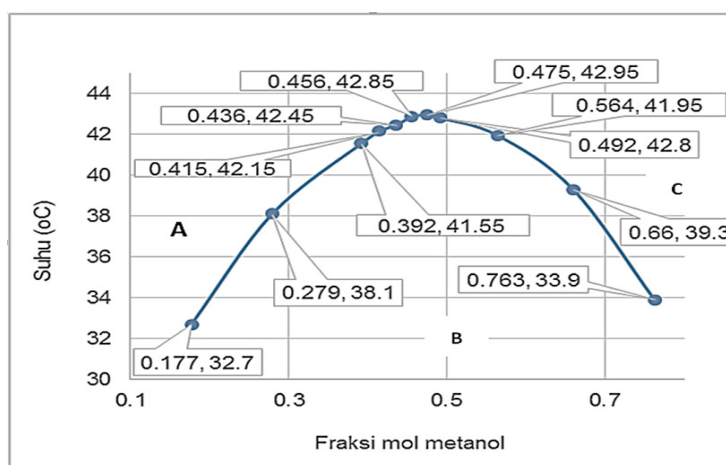
The results obtained from the addition of a certain amount of methanol into a 5 ml n-hexane are presented in Table 2.

**Table 1.** Density, molar mass, and boiling point of n-hexane and methanol

Substance	Density (g/ml)	Molar mass (g/mol)	Boiling point (°C)
n-hexane	0.660	86.18	69.0
Methanol	0.792	32.04	64.7

**Table 2.** Temperature of the mixture of 5 ml n-hexane with methanol addition

Volume of methanol (ml)	Average temperature (T) (°C)	Methanol mass (gram)	N-hexane mass (gram)	Mole Fraction of methanol	Mole fraction of n-hexane
0.1	Clear solution (methanol was dissolved in n-hexane) at 26°C				
0.2	Clear solution (methanol was dissolved in n-hexane) at 26°C				
0.3	Clear solution (methanol was dissolved in n-hexane) at 26°C				
0.4	32.70	0.2640	3.3	0.177	0.823
0.6	38.10	0.4752	3.3	0.279	0.721
1.0	41.55	0.7920	3.3	0.392	0.608
1.1	42.15	0.8712	3.3	0.415	0.585
1.2	42.45	0.9504	3.3	0.436	0.564
1.3	42.85	1.0296	3.3	0.456	0.544
1.4	42.95	1.1088	3.3	0.475	0.525
1.5	42.80	1.1880	3.3	0.492	0.508
2.0	41.95	1.5840	3.3	0.564	0.436
3.0	39.30	2.3760	3.3	0.660	0.340
5.0	33.90	3.9600	3.3	0.763	0.237

**Figure 1.** The correlation curve of mole fraction of methanol to temperature in n-hexane-methanol phase diagram.**Diagram of n-hexane and methanol system**

Based on the data in Table 2, the curve in phase diagram of the interaction between methanol mole fraction with temperature could be constructed (Figure 1).

Based on Figure 1, the asymmetrical-shaped curve (tend to skew to the right) shows the solubility of n-hexane in methanol that is relatively small compared to the solubility of metha-

nol in n-hexane. This is due to the solubility of a substance that is also influenced by the size of the solute hydrocarbon chain. The longer the hydrocarbon chain, the smaller the solubility of the solute. Continuous chain molecules such as n-hexane open chain, can straighten the molecules according to the chain winding (zig-zag), which allows the atoms of the molecules occupy a position that corresponds to the radius of van der

Waals. Maximum towing of van der Waals arises between the molecules of n-hexane. Therefore, more energy is needed to overcome the van der Waals towing between molecules of n-hexane resulted in the smaller solubility (Fessenden & Fessenden, 1986).

Based on Figure 1, methanol and n-hexane can dissolve each other at any given composition when the system temperature was above 42.95 °C. This temperature is called as the maximum critical temperature (consolute temperature) of the n-hexane-methanol system with  $X_{\text{methanol}} = 0.475$  ( $P = 715$  mmHg). The obtained maximum critical temperature was closed to the results obtained in Rothmund (in Alessi et al, 1989) that was equal to 43.5 °C. However, these results were not consistent with the results obtained by Alessi et al (1989) that was equal 35.15 °C. The differences in the results obtained were thought to be caused by the presence of water in methanol (purity level of methanol). This study used methanol with a density of 0.792 g/ml. According to the results of the research of Alessi et al (1989) about the density of methanol-water system as a function of the mole fraction of water at 298.15 K; it showed a mole fraction of the water with a density of methanol amounted to 0.792 g/ml around 0.0349. Meanwhile, the methanol used by Alessi et al, (1989) had a density of 0.786846 g/ml and showed 99.9% purity of methanol. Thus, the presence of water in methanol could affect the data of liquid-liquid equilibrium of the n-hexane-methanol binary system obtained.

#### Mental model of n-hexane-methanol system

The submicroscopic level visualization of the interaction that occurred in the n-hexane and methanol mixture is presented in Figure 2.

#### Single-phase of N-hexane-methanol system (region A)

Methanol is a polar substance that is polar (dipole moment 1.69 D) while the n-hexane is a non-polar substance (dipole moment 0.08 D). Between the methanol molecules, there is an interaction in the form of hydrogen bonds. Meanwhile, the interaction between molecules of n-hexane occurs through London force. Molecularly, the hydrogen bond is stronger than the London force.

When methanol is added to the n-hexane, London force between then-hexane molecules and the hydrogen bonds between the methanol molecules will be disconnected. A new interaction between n-hexane and methanol will be formed. However, the new interaction formed is different with the previous interaction. The energy required to break the hydrogen bonds is greater than the energy needed to alter the London force. Methanol molecules must compensate for losing some of the hydrogen bonds and the formation of a weak interaction between n-hexane and methanol with new form of hydrogen bonds in a new setting. The interaction in the system after mixing n-hexane with methanol is proportional to the strength of the interaction of each substance in a separate state. For this reason, a small amount of energy is absorbed when a small amount of methanol can be dissolved in n-hexane, or vice versa.

The low solubility of methanol in n-hexane or vice versa can be explained by the change in the entropy of the system. When n-hexane is mixed with methanol, the particles formed by the new arrangement shows the lower entropy of system than the entropy of each fluid (methanol and n-hexane) in a separate state. Naturally, there is a tendency toward entropy methanol and n-hexane in a separate state (higher entropy of the system); therefore, both the liquid is difficult to mix (so-

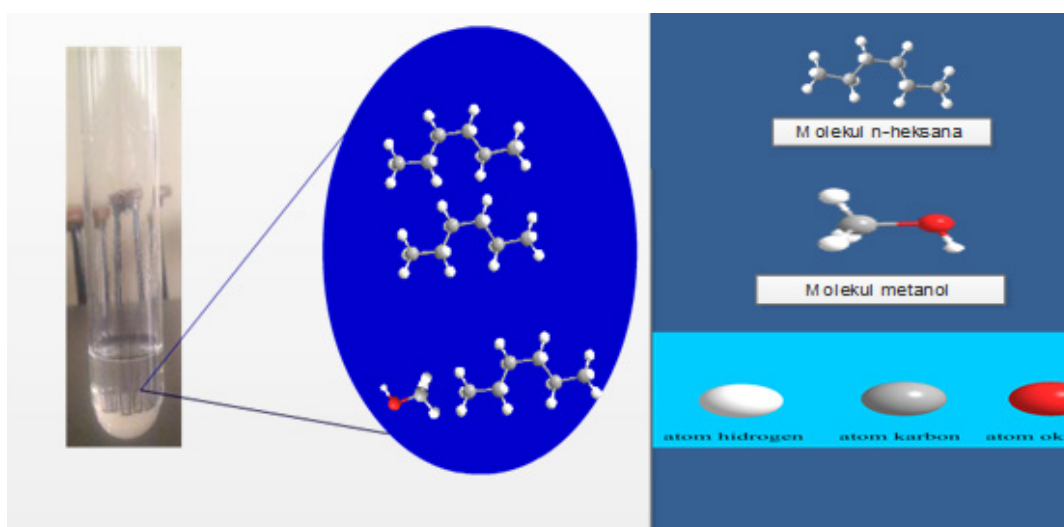


Figure 2. Mental model of a single-phase of n-hexane-methanol system in the region A of the curve



lution becomes cloudy and form a two-phase). Possible interaction between the molecules of n-hexane and methanol molecules is London force. The hydrogen atoms of the methyl group (hydrocarbon) in methanol molecules will interact with hydrogen atoms from n-hexane molecules. In addition, the region A of this curve shows an interaction between the n-hexane molecules in the form of London force, the interaction is visualized in Figure 2.

*Single-phase of n-hexane-methanol system (region C)*

The relationship curve between temperatures with n-hexane-methanol composition showed that the region C is the area of a single-phase. It means that there is a dissolution process when adding a certain amount of n-hexane into methanol at a certain temperature and air pressure at 715 mmHg. Figure 3 shows the methanol molecules can bind to the molecules of n-hexane through London force. Meanwhile, among other methanol molecules is formed the hydrogen bonds.

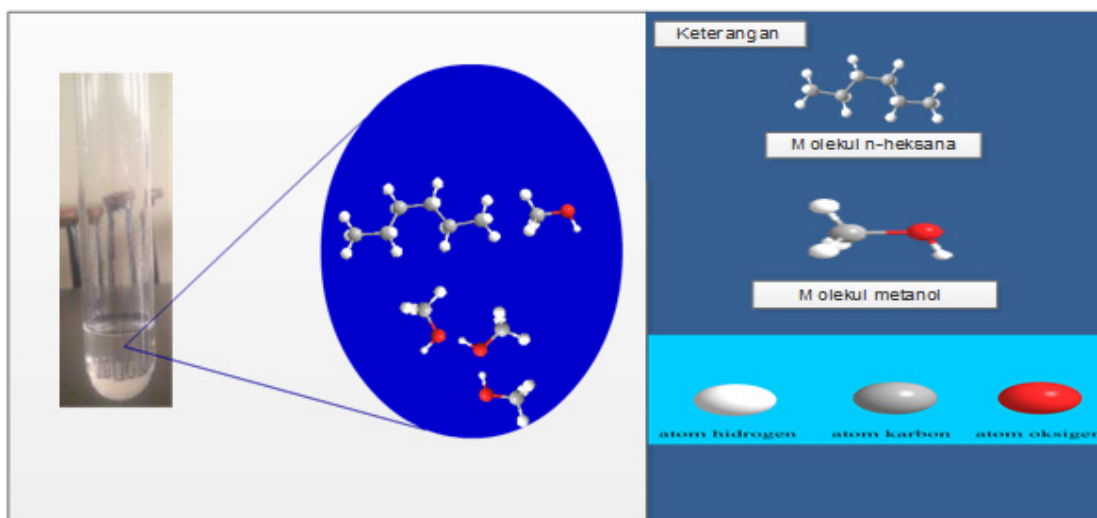
*The addition of 1.5 ml methanol into 5 ml n-hexane to form a two-phase (region B)*

Mixing 1.5 ml methanol into 5 ml n-hexane produced a two-phase (two layers). This result showed shows the limitation of solubility of methanol in n-hexane. According to the density of both substances, the majority of n-hexane was on the top layer, while the majority of the methanol was in the bottom layer. Figure 4 shows the interaction of London force between methanol and n-hexane molecules and the interaction of London force between n-hexane molecules at layer 1 (the top layer). Meanwhile, at layer 2 (bottom layer), the interaction between n-hexane molecules is in the form of London forces and the interactions between methanol molecules is in the form through hydrogen bonds.

*N-hexane-methanol system in a single-phase above the curve*

Increasing of the system temperature until it reached a critical temperature could accelerate the process of methanol dissolution in n-hexane. This was because of the great thermal movement resulted in greater mixing capabilities in both components. The increasing of the system temperature resulted in a number of energy absorbed by the system altered the interactions (the intermolecular attractive force), which acted between n-hexane and methanol molecules. The entropy of the system was increased. As a result, the mixing ability of the two substances was greater. The mixing of methanol and n-hexane above the maximum critical temperature resulted in the n-hexane-methanol dissolution process could take place in any composition. Figure 5 is an example of the interaction between n-hexane and methanol molecules through London forces in addition to the interaction between n-hexane molecules through London force as well.

The phase formula of n-hexane-methanol system at a constant pressure is  $f = c - p + 1$ . The degrees of freedom ( $f$ ) for the region in two phases (region B in the curve), which consists of two components, namely the n-hexane and methanol is  $f = 1$ . It only needs one variable to declare a state of the system in this region. If the selected variable is the temperature of the system, then the tie line with the curve of the second composition resulting in a conjugate solution (methanol in n-hexane and n-hexane in methanol). If the selected variable is the composition of a solution of the conjugate, then the system temperature and the other solution composition can be determined. Meanwhile, the degrees of freedom for the region of the phase (regions A and C on the



**Figure 3.** Single-phase of n-hexane-methanol system (region C)

curve and the region above the curve) is  $f = 2$ . It is indicated that it takes two variables to declare a state of the system in this area. If the selected variable is the composition of a conjugate solution and the system temperature then other conjugate composition of the solution can be determined.

#### The overview of standpoint of thermodynamics (chemical potential) phase equilibrium of the n-hexane and methanol system

Macroscopically, we can observe only two possibilities when the two liquids are mixed, i.e. a single-phase or a two-phase. The first possibility occurs when the solubility of the first liquid in the second liquid has not been exceeded. The second possibility occurs when the solubility of one of the liquids are exceeded and hence will occur in two phases, each of which is a saturated solution. Both possibilities can be explained from the

standpoint of thermodynamics than the explanation on the submicroscopic level with respect to the intermolecular attractive forces that have been described previously. When methanol is dissolved in n-hexane, then methanol in the chemical potential of the solution can be expressed as  $\mu$ .  $\mu^0$  is the chemical potential of methanol in a pure state, whereas  $x$  is the mole fraction of methanol in the solution with the assumption of an ideal solution. If the chemical potential of methanol in n-hexane is lower than the chemical potential in a state of pure methanol, the dissolution process may still be ongoing. However, after the leaching process is beyond the point, the chemical potential of methanol in the solution is greater than the chemical potential in a state of pure methanol; the methanol transfer will occur to the outside of the solution entering the pure methanol phase and eventually reach the equilibrium state.

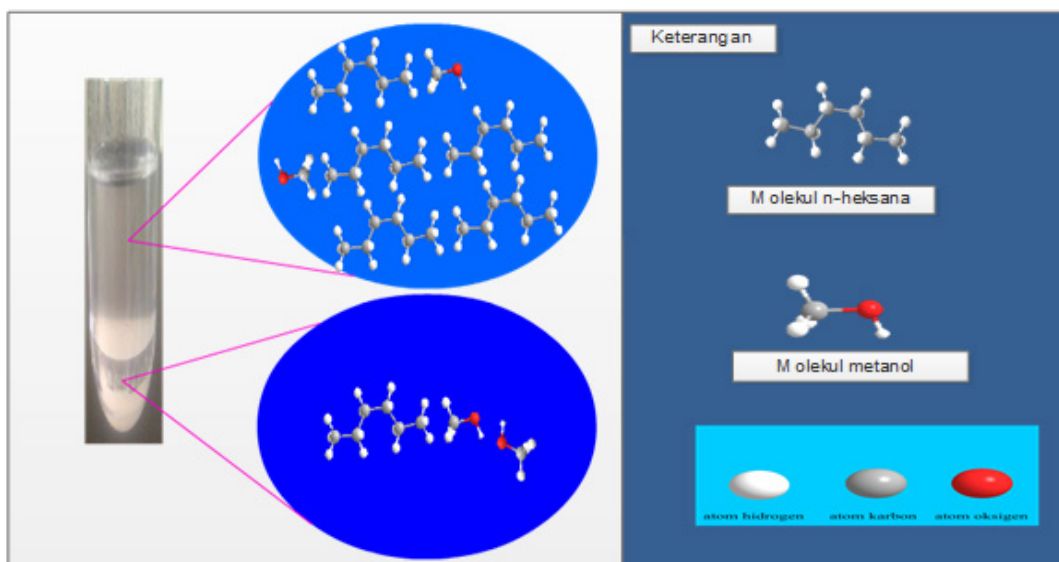


Figure 4. Mental model of a two-phase of n-hexane-methanol system in the region B of the curve

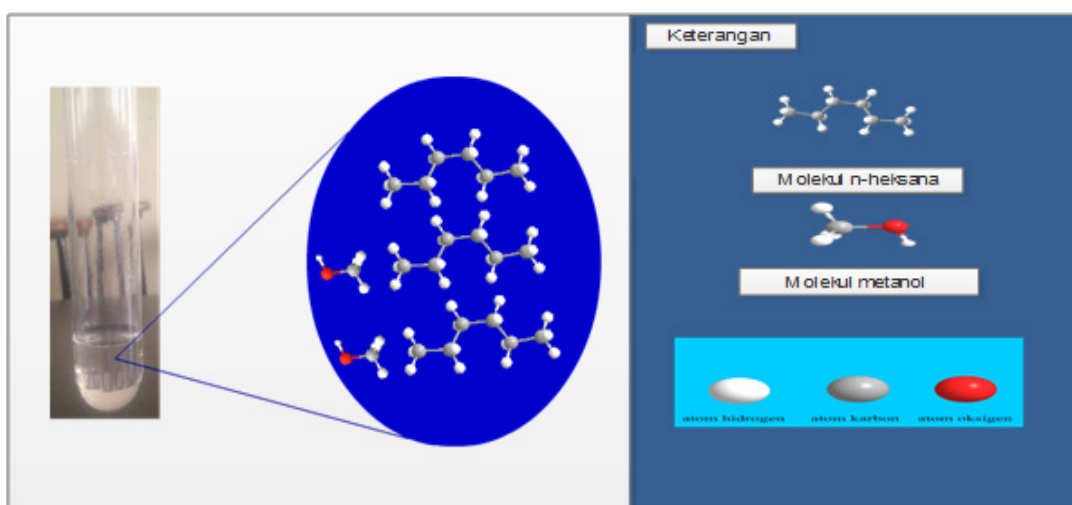


Figure 5. Mental model of n-hexane-methanol system in single-phase above the curve

This explanation can also be applied to explain the second component is n-hexane. If the chemical potential of n-hexane in the solution is lower than the chemical potential of pure n-hexane, then the dissolution process of n-hexane in methanol is still ongoing. However, if a potential chemical of n-hexane in the solution is greater than the potential of n-hexane in a state of pure, then the displacement components of n-hexane out of solution will be occurred and entering into the pure phase of n-hexane. After reaching the equilibrium state, both saturated solution, i.e. methanol in n-hexane and n-hexane in methanol are called conjugate solution. Thus, the two phases are in equilibrium; therefore, there are no one of two phases is in a pure substances phase. At equilibrium (area B on the curve), the chemical potential of each component in the phase are the same. Suppose that the first phase is symbolized by  $\alpha$  and the second phase is symbolized by the  $\beta$  then it can be expressed as (Alberty & Daniels, 1981).

Overall, the mental model of this binary system describes the interactions that occur at the submicroscopic level of mixing n-hexane and methanol according to the definition of mental models that are synthesized from the opinion of some experts. Mental model is an internal representation of cognitive constructed by someone; include a visual-pictorial component and propositional components to understand or to give a rational explanation of a real-world phenomenon or imaginary situations, events, or processes. The structure reflects the structure of which can be felt (perceived structure) on those situations, events or processes (Schnotz & Bannert in Wang & Barrow, 2010); Nersessian in Tumay, 2014).

This binary system study showed that n-hexane and methanol can be mixed at a certain temperature and composition. The macroscopic phenomenon of n-hexane and methanol mixing in four areas of system curve can be explained in submicroscopic level regarding to the interactions that occur in the system. Tversky in Akaygun & Jones (2013) stated that the image is an effective cognitive tool when it used as a concrete and meaningful representation. It is more effective compared to the written language. On the other hand, written language is more effective to communicate and to deliver the abstract concepts, causality and quantification. It is difficult to illustrate these concepts in pictorial. The findings in this study were able to accommodate these two ideas. The phenomenon of binary system of n-hexane-methanol was described by using visualization and verbal explanation.

The concept of polarity and intermolecular towing force is a pre-requisite concept that students must master it in order to explain the submicroscopic level of observed binary system phenomena. In addition, the concepts of thermodynamics (e.g. chemical potential and entropy) are required to describe the symbolic level of observed binary system phenomena. On the other hand, the results of the research on atomic structure, periodic system of elements, chemical bonding, molecular geometry and polarity shows the quality of the students on explaining the material of study in these topics were varied from high to low abilities, in line with their ability to reconcile the new information into the frame of existing knowledge (Wang & Barrow, 2013). Students have the alternative conceptions of intermolecular and intramolecular towing forces (Sendur, 2014). In addition, the results of an investigation of 34 students with varying alternative conceptions about chemical thermodynamics indicated that this material was not easy to learn because it is too abstract (Sreenivasulu & Subramaniam, 2013).

In summary, the study of the mental model of n-hexane-methanol binary system was very useful to the formation of mental model and it increased the understanding of the student of chemistry teacher candidate. The ability to construct and to use the mental models could affect the conceptualization of students about the chemistry concepts on the topic of the binary system. In line with the opinion of Wang & Barrow (2010) who stated that the student of teacher candidates were needed to be encouraged to use mental model as a tool for linking the three levels of chemical representation when inserting knowledge into long-term memory (Devetak, Vogrinc & Glazar in Jansoon et al., 2009). According to this result, in order to support the efforts to develop a basic understanding of chemistry concepts, the learners should be able to associate their understanding in the level of symbolic to the level of macroscopic and the level of submicroscopic (Bain et al., 2014; Hernandez et al., 2014). It certainly needs to be supported by the pattern of teaching facilities which are useful for generating discussion connectedness between levels of representation (Becker et al., 2015).

## CONCLUSION

The study of mental model of n-hexane-methanol binary system could be in the form of visualization of intermolecular interactions that occur between n-hexane and methanol through

London forces; also in the form of intermolecular interactions between methanol through hydrogen bonds and intermolecular interactions of n-hexane through London force. Mental model of the system was described in the four areas curve of methanol mole fraction to the temperature in a phase diagram of n-hexane-methanol system. Based on the curve of the system phase diagram, methanol and n-hexane could dissolve each other at any given composition when the system temperature was above 42.95 °C. This temperature was called as the maximum critical temperature (above consolute temperature) of n-hexane-methanol system. The results of the mental model study of n-hexane-methanol binary system can be followed up by developing a learning model of binary systems to improve the mental model and the student understanding.

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