Malaysian Journal of Science **26** (2): 91 – 98 (2007)

Effect of Isocyanate Index on Physical Properties of Flexible Polyurethane Foams

C. S. Lee[1, 2 *], T. L. Ooi[2], C. H. Chuah[1] and S. Ahmad[2]

[1] Department of Chemistry, Faculty of Science, University of Malaya, Lembah Pantai 50603 Kuala Lumpur, Malaysia

* leechoysin79@yahoo.co.uk (corresponding author)

[2] Advanced Oleochemical Technology Division, Malaysian Palm Oil Board, P.O. Box 10620, 50720 Kuala Lumpur, Malaysia.

Received 8th January 2007, accepted in revised form 25th July 2007.

ABSTRACT Water blown flexible polyurethane foams were made based on ratio 1:1 (w/w) mixture of palm oil-based polyester polyol with number average molecular weight (Mn) of 5000 and commercial polyether polyol with molecular weight of 5000, 2.14 pph water and varying amounts of toluene diisocyanate (TDI). The effect of isocyanate index on the physical properties of flexible polyurethane was investigated. Isocyanate index of 100 produced the highest density foam (60.6 Kg/m^3) with the lowest hysteresis (23.8%), good tensile strength (0.0995 MPa) and tear resistance (0.2468 N/mm).

ABSTRAK Busa lembut adalah dibuat berdasarkan campuran 1:1 poliol minyak kelapa sawit yang nombor jisim molekul puratanya 5000 dengan komersial poliol yang jisim molekulnya 5000, 2.14 pph air dan kuantiti toluene isosianat yang berlainan. Kesan daripada indeks isosianat pada sifat fizikal poliuretana lembut telah diselidik. Keputusan menunjukkan indeks isosianat 100 menghasilkan busa yang paling tumpat (60.6 Kg/m^3) dengan 'hysteresis' yang paling rendah (23.8%), ketegangan (0.0995 MPa) dan ketahanan koyak (0.2468 N/mm) yang lebih baik.

(Compression stress, density, elongation at break, flexible polyurethane, hysteresis, isocyanate index, tear resistance, tensile stress)

INTRODUCTION

The first commercial flexible polyurethane foam was produced in Britain in 1954 [1]. These foams are playing important roles in many industries, such as roof material and seat cushion for cars, aircrafts and trains, cushion for bed, sofa and other furniture, soft sole for shoes and others. The global polyurethane market in 2004 showed that flexible polyurethane foams contributed the most to the market, which was 47%, followed by rigid foam insulation (26%), and others (27%) [2]. Flexible polyurethane foams meet most of the requirements for cushioning in furniture, bedding and automotive. The potential flexible polyurethane markets are no doubt in a leading position.

A lot of work has been done to improve the flexible polyurethane foam [3 - 8]. Polyurethane foams can be improved by using different polyol, such as synthetic polyether, polyester polyol that derived from petroleum and various vegetable oils with different molecular weight. Besides, alterations in foam formulations by using different amount and type of additives and blowing agents will produce different properties foam. In this work, we studied the isocyanate index on the properties of flexible polyurethane foams.

MATERIALS AND METHODS

Materials

Palm oil-based polyester polyol with number average molecular weight (Mn) of 5000 (Hydroxyl value = 32.78 mgKOH/g sample) and commercial polyether polyol with molecular weight of 5000 (Hydroxyl value = 38.12 mgKOH/gsample) was obtained from AOTD, MPOB. Additives: NIAX stannous octoate catalyst (G.E. Silicone), NIAX A33 triethylenediamine (TEDA) catalyst (G.E. Silicone), NIAX dimethylethanolamine (DMEA) cross-linker (G.E. Silicone), Niax silicone surfactant L580 (G.E. Silicone) and toluene diisocyanate (TDI) (Miliken Chemical), of industrial grade were used as purchased.

Foam Preparations and Evaluations

Equivalent ratio 1:1 (w/w) of palm oil-based polyester polyol with number average molecular weight (Mn) of 5000 and commercial polyether polyol with molecular weight of 5000, stannous octoate catalyst, TEDA catalyst, DMEA cross-linker, silicone surfactant and water as blowing agent were mixed together in a plastic cup and stirred vigorously at 8000 rpm by a mechanical stirrer until the mixture became creamy. After that, the stirring was stopped before adding TDI and the stirring process continued at the same speed for another 10-15s. The liquid mixture was then poured into a plastic box (18 X 12 X 8 cm) and left to rise and cured at room temperature (25°C) for 7 days before all the mechanical measurements were carried out.

Density measurement

The test specimens (100mm X 100mm X 50mm) were weighed to determine the density in kilograms per cubic meter. Three specimens were tested and the average value was reported.

Compression stress and hysteresis test

The test was conducted according to DIN 53577 Compression of Flexible Cellular Materials Test. Foams with dimension 50mm x 50mm x 50mm were compressed between two flat plates at the speed rate of 100mm/min. The instrument used was Zwick Universal Testing Machine with crosshead monitor and compression platens as the grip. Based on the stress against strain curve graph, compressive stress and hysteresis were recorded. Hysteresis is the ability of foam to maintain its original support characteristics when stress is applied. Lower hysteresis values indicate less energy loss and better foam durability [9].

Tensile stress and elongation at break

The test was conducted according to ASTM

D3574 Foam Tension Test E. Foams were cut to flat sheets with 12.5 ± 1.5mm thickness and cut into dumbbell shape according to Test Methods D 412. The test was conducted by using Zwick Universal Testing Machine. The specimens were gripped by two screw-type flat plate grips and pulled at a speed of 500 ± 50mm/min. The tensile stress and the elongation at break were recorded.

Tear resistance test

The test was conducted according to ASTM D3574 Foam Tear Resistance Test F. The foam specimens were cut to the shape that shown in Figure 1. The specimens were clamped to the jaws of the test machine, Zwick Universal Testing Machine. The specimen block was pulled by the jaw diagonally at the speed of 500 ± 50mm/min. Maximum force was recorded and the tear strength was calculated as follows:

Tear Strength, N/mm= F/T

Where, F= force, N

T= thickness, mm

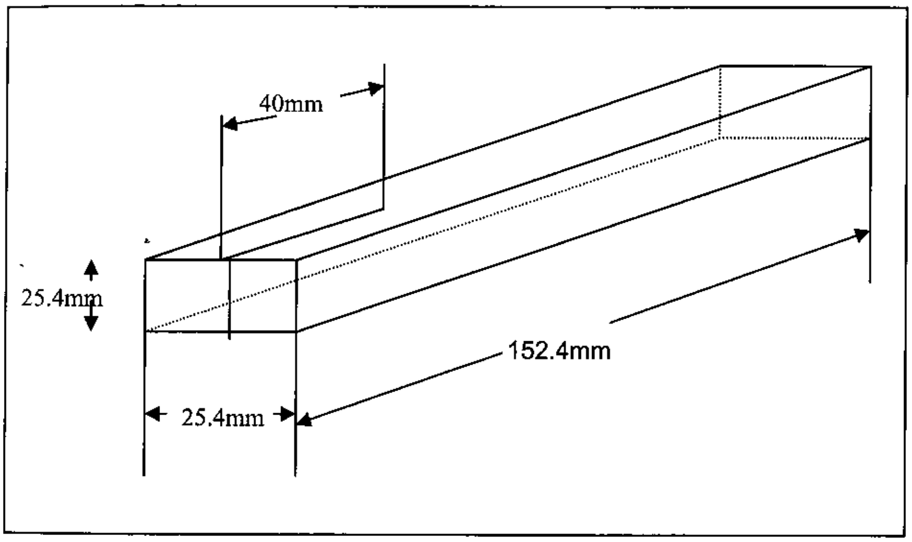

Figure 1. Tear resistance test specimens

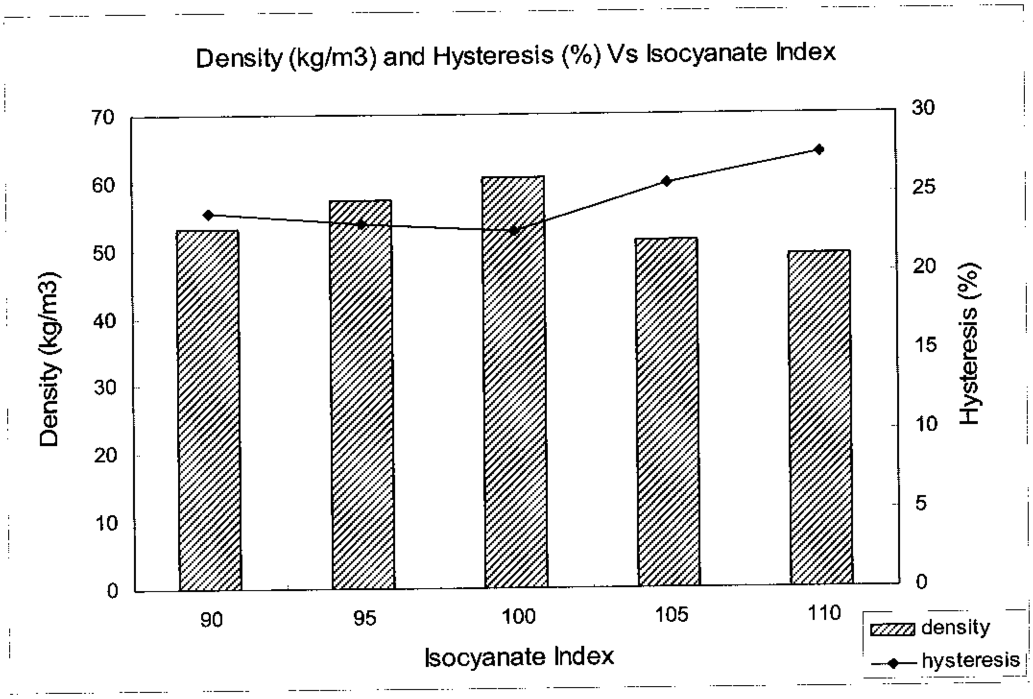

Figure 2. Effect of isocyanate index on foam density and hysteresis

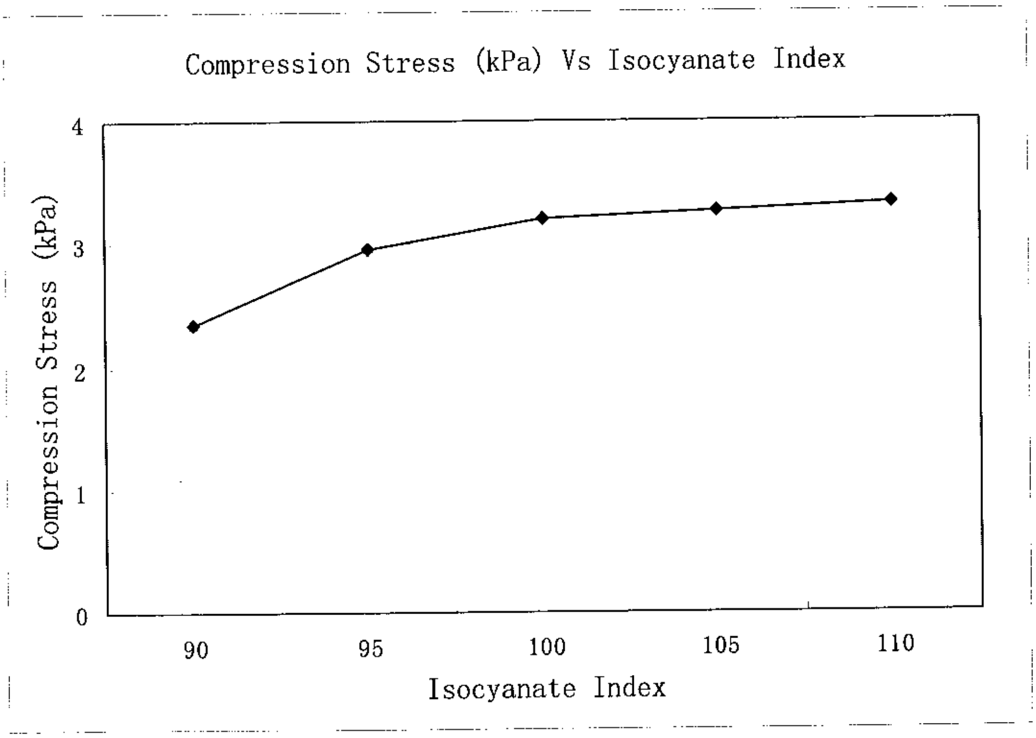

Figure 3. Effect of isocyanate index on foam compression stress (KPa)

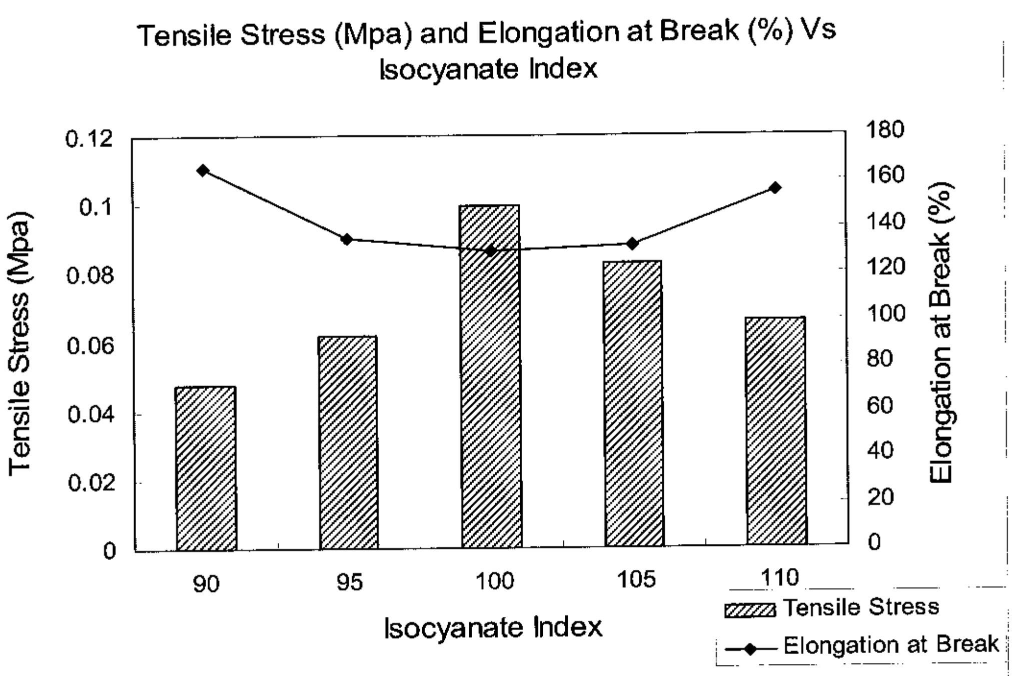

Figure 4. Effect of the isocyanate index on foam tensile stress (MPa) and elongation at break (%)

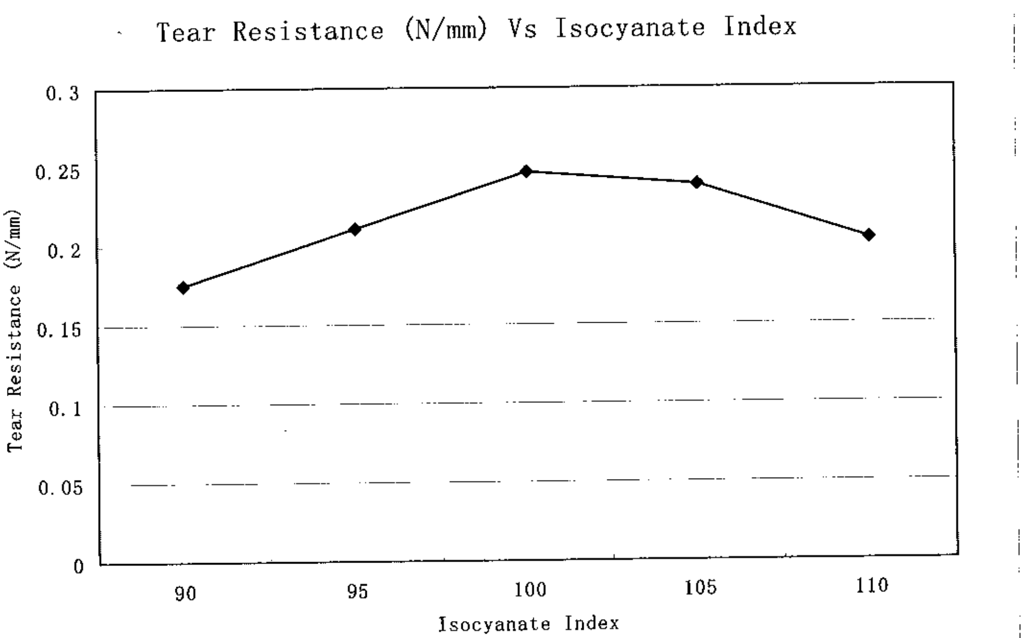

Figure 5. Effect of isocyanate index on tear resistance

RESULTS AND DISCUSSION

Flexible polyurethane foam was prepared by using ratio 1:1 (w/w) palm oil-based polyester polyol with number average molecular weight (Mn) of 5000 and commercial polyether polyol with molecular weight of 5000. Alteration in the foam formulation such as varying the amount and type of polyols, catalysts, cross-linkers, surfactants and blowing agents will result in different quality of foams. Studies were done on the effect of diethanolamine and toluene diisocyanate index on the morphology and structure of flexible foams [10, 11]. Norin *et al.* have also studied on the influence of stannous octoate catalyst to the physical properties of flexible polyurethane [12].

In this study, we used a typical formulation to study the effect of isocyanate index on the physical properties of the foam (Table 1). The isocyanate index was varied from 90 to 110. The isocyanate index is the amount, in percentage, of isocyanate used divided by the amount of isocyanate required to react with all reactive species that took part in the reaction [13]. Figure 2 shows of the effect of isocyanate index on density and hysteresis of the foams. There is a co-relation between the density and the hysteresis of the foam. Higher density foams have lower hysteresis than lower density foams. Foams made using isocyanate index of 100 possess the highest density, which is 60.6 kg/m^3 but its hysteresis is the lowest, which is 23.8%. Higher density foam can bear major stresses with minimum strain than the lower density foam. Hence, higher density foams provide more comfort and longer service life to users [13].

The increment of isocyanate index from 90 to 100 caused an increment of foam density but when the isocyanate index was increased from 105 to 110, a reduction of foam density occurred. This may be due to high excess of the isocyanate index ranging from 105 to 110 which decelerated the competition between water and other active hydrogen compounds to react with isocyanate. Therefore, the amount of isocyanate became less crucial in this situation. The reaction between isocyanate and water will form carbamic acid that further reacts to give urea and carbon dioxide [15]. The surplus carbon dioxide will blow up the polyurethane foam and consequently produce lower density foam.

The compression stress of the foam increased proportionately with the isocyanate index from 90 to 110 (Fig. 3). Figure 4 shows the effect of isocyanate index on tensile stress and elongation at break. Foams made with isocyanate index of 100 produced the strongest tensile stress but the weakest elongation, which were 0.0995 MPa and 129.9% respectively. The tear resistance of the foam was found to increase with higher isocyanate index, but this only limited between 90 to 100 indexes (Fig. 5). This indicated maximum strength of tear resistant and tensile stress by utilizing the isocyanate index of 100 in foams production.

Table 1. Typical Formulation for Flexible Polyurethane Foam

COMPONENT A	PART (pph)
Palm Oil-based Polyester Polyol	50
Commercial Polyether Polyol	50
Stannous Octoate Catalyst	0.08
TEDA Catalyst	0.57
DMEA Cross-linker	1.00
Silicone Surfactant	1.00
Blowing Agent (distilled water)	2.14
COMPONENT B	**PART (pph)**
Toluene Diisocyanate	26.9
Isocyanate Index	100

ACKNOWLEDGEMENTS

This work was supported by the MPOB Graduate Research Grant.

REFERENCES

1. Buist, J. M., Ball, G. W. and Woods, G. (1970). Flexible foam: Manufacture and properties. In: *Advances in Polyurethane Technology.* (eds. Buist J. M. and Gudgeon, H.). Elseivier Publ. London and Amsterdam, pp. 141 - 186.
2. Kerman, M. L. (2001). A snapshot of the global polyurethane market and the future of nature based polyurethane raw materials. *Proceedings of the Oleo and Specialty Chemicals Conference PIPOC 2005 International Palm Oil Congress*. pp. 334 - 344.
3. Campbell, G. A. (1979). Compressive creep of flexible polyurethane foam. *J. Applied Polymer Sci*. **24**: 709 - 723.
4. Lin, Y., Hsieh, F. and Huff, H. E. (1997). Water-blown flexible polyurethane foam extended with biomass materials. *J. Applied Polymer Sci*. **65**: 695 - 703.
5. Kaushiva, B. D., Dounis, D. V. and Wilkes, G. L. (2000). Influences of copolymer polyol on structural and viscoelastic propreties in moulded flexible polyurethane foams. *J. Applied Polymer Sci*. **78**: 766 - 786.
6. Javni, I., Petrovic, Z. S., Guo, A. and Fuller, R. (2000). Thermal stability of polyurethanes based on vegetable oils. *J. Applied Polymer Sci*. **77**: 1723 - 1734.
7. John, J., Bhattacharya, M. and Turner, R. B. (2002). Characterization of Polyurethane Foams from Soyabean Oil. *J. Applied Polymer Sci*. Vol. **86**: 3097 - 3107.
8. Monteavaro, L. L., Silva, E. O., Costa, A P. O., Samios, D., Gerbase, A. E. and Petzhold, C. L. (2005). Polyurethane networks from formiated soy polyols: Synthesis and mechanical characterization. *J. Am. Oil Chem. Soc.* **82**: 365 - 371.
9. Verhelst, G. and Parfondry, A. (1970). Introduction to flexible foams. In: *The Polyurethanes Book.* (eds. Randall, D. and Lee, S.) John Wiley & Sons. United Kingdom. pp. 180 - 181.
10. Dounis, D. V. and Wilkes, G. L. (1997). Influence of diethanolamine on hard segment ordering in flexible polyurethane foams. *J. Applied Polymer Sci*. **65**: 525 - 537.
11. Dounis, D. V. and Wilkes, G. L. (1997). Effect of toluene diisocyanate index on morphology and physical properties of flexible slabstock polyurethane foams. *J. Applied Polymer Sci*. **66**: 2395 - 2408.
12. Shaari, N. Z. K., Ooi, T. L., Ahmad, S., Siwayanan, P., Ang, P. F., Wiese, D. and Tan, W. I. (2001). Palm-based flexible polyurethane foams. *Proceedings of the PIPOC 2001 International Palm Oil Congress (Oleochemicals)*. pp. 130 - 135.
13. Wirpsza, Z. (1993). *Polyurethanes: Chemistry, technology and applications.*

Ellis Horwod Publ. Great Britain. pp. 97 and pp. 226 - 252.

14. Johnson, P. C. (1970). Isocyanate reactions: Nature, control and significance in manufacture of polyurethanes. In: *Advances in Polyurethane Technology.* (eds. Buist, J. M. and Gudgeon, H.). Elseivier Publ. London and Amsterdam, pp. 1 - 23.
15. Saunders, J. H. (1978). *Polyurethanes Chemistry and Technology Part I: Chemistry.* Robert E. Krieger Publishing Company. New York, pp. 76 - 79.