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Development of Chemical Proportion Formulation Model for Quality Control in Flexible Polyurethane Foam Production.

Akingbade K. F.

Department of Electrical & Electronics Engineering ,The Federal University of Technology, Akure, Nigeria.

Key words:
Flexible Polyurethane foam, Chemical Proportion Formulation, Quality Control

A B S T R A C T

A major section involved in the production of flexible polyurethane foam (FPF) is the chemical proportion formulation. This section determines the quality of the foam to be produced. Quality control in FPF production cut across this section, as wrong chemical formulation yields a different foam as compared to the desired foam. This work developed a model capable of generating chemical formulation for a specified foam density. Chemical formulations for four different foam densities were obtained and compared with manual real life data obtained from a foam manufacturing industry located in the North Central part of Nigeria. Using a two-sample t-test, the result shows that there is no significant difference between the model result and the real life data. 2-tailed significance of 0.215, 0.088 and 0.124 were obtained for polyol, TDI and water respectively and were seen to be greater than the level of significance (0.05)

1. Introduction

Flexible polyurethane foam (FPF) is one of the most vital classes of cellular plastic from mixture of different chemicals, this cellular plastic are used in producing pillows, furniture, foam mattresses, carpet underlay, cushioning material used in automobile [8,10]. FPF is ideal for these purposes due to its resilience, durability, comfort, support and other favorable properties [11]. Its other area of application is shown in Fig. 1.

Owing to the large area of its application, quality control has become a major task for FPF producers. According to [2] it is believed that a company without quality control offer no economic benefits. Since quality control cut across preproduction processes in process industry, therefore it is important that quality control strategy be introduced to chemical proportion formulation in FPF production because it's one of the preproduction processes that determines the quality of FPF to be produced. Therefore, a precise system that can generate chemical proportion formulation for a specified foam density is highly needed in FPF production to eliminate possible human errors. This work developed a model capable of determining chemical proportion formulation and provides a graphical user interface (GUI) for the user.

Correspondence:
E-mail address: kfakingbade@futa.edu.ng, kfakin@mit.edu

In synthesizing flexible polyurethane foam there are many different components needed, the seven major ones are Polyol, Isocyanate (Toluene-Di-Isocyanate), water, Amine, Stannous Octoate, Silicone oil and Methylene Chloride [9]. In the production of flexible polyurethane foams, each of the chemicals/components being used has its own properties and roles in the production process.

Polyol is an almost colourless and odourless high viscous liquid [5]. Majorly polyols come in two types, which are polyether polyol and polyester polyol depending on the production method [4]. The most used type of polyol is the polyether polyols; around 90% of flexible polyurethane foam manufacturers all over the world use it [3-5]. In the production of flexible polyurethane foams, polyol is a major chemical that forms the backbone of the polymer chain [4, 5], which means the quality of the polyol used will affect the overall quality of the foam produced.

2. Methodology

2.1 *FPF Components and Functions*

In synthesizing flexible polyurethane foam there are many different components needed, the seven major ones are Polyol, Isocyanate (Toluene-Di-Isocyanate), water, Amine, Stannous Octoate, Silicone oil and Methylene Chloride [9]. In the production

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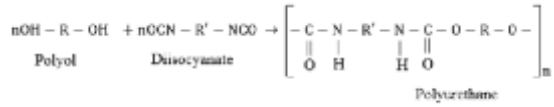

(1)

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In the production of flexible polyurethane foams the most commonly used isocyanate is Toluene-Di-Isocyanate (TDI), mostly the mixture of the two polymers is in the ratio 80:20 (2,4 –Toluene diisocyanate and 2,6-Toluene diisocyanate) [5]. It exists as colourless to pale yellow liquid with a pungent odor, is a low viscous liquid [5, 7], it decomposes in water and soluble in some chemicals such as acetone and benzene [7]. It participate in the formation of CO_2 by reacting with water and the curing process, which in turn determine the hardness of the foam [5].

Polymers containing urethane linkage is termed polyurethanes, this urethane linkage is –NH-CO-O [12]. PU is formed by a chemical reaction containing at least two isocyanates functional group with compounds that have active hydrogen, such as diols, that contain two or more hydroxyl groups in the presence of a catalyst, chain extender and/or other additives [12, 13, 14].

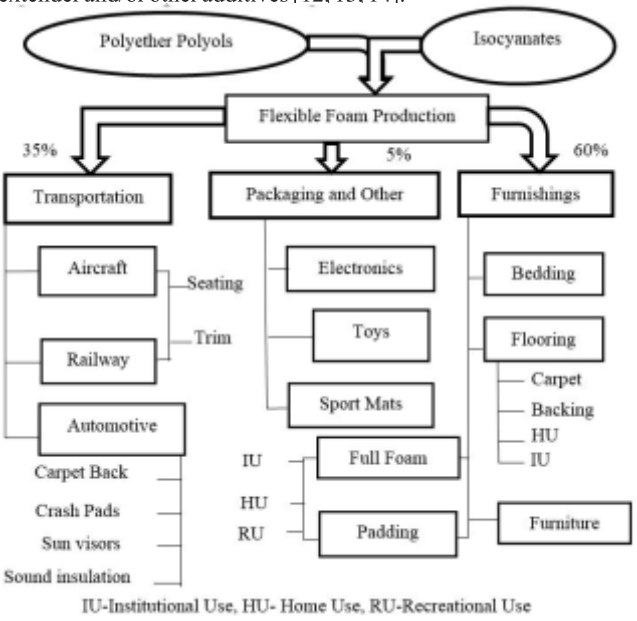
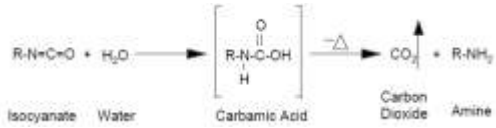


Fig. 1: Application of flexible polyurethane foam [2]

The chemical equation between polyol and isocyanate is as shown in (1). The product of this reaction is a basic material whose variation can be stretched, smashed, or scratched, and without affecting the originality of the basic material, this characteristic allows PU to be modified to suit a specific need by reacting appropriate compounds [4, 12]. PU can take different forms depending on the difference in isocyanate and polyol constituents, it can be liquid, foam or solid [4]. PU is an exceptional material that proffers the elasticity of rubber coupled with the toughness and durability of metal [4]. PU is typically thermoplastic and thermoset in nature, which means, it is hard to melt and recycle [13, 14]. Flexible polyurethane foams are produced from linear or high molecular weight polyols that contain few hydroxyl groups per molecule, which on reaction with isocyanate gives structures with low degree of cross-linking[15]. Its production is basically based on the controlled expansion of gas during polymerization process [8].

Water is one of the important elements used in the production of flexible polyurethane foams. The reaction of water with isocyanate is termed the blow reaction and is a two-step process [2], it produces polyurea, carbon dioxide (CO_2) and heat as shown in (2).



(2)

The gas (CO_2) that is produced plays a large role in blowing the liquid into foam when it diffuses with the existing gas bubbles in the polyol [2, 16]. The cell structure and the solid state morphology of the foam are influenced when the water content in the production is increased as well as the blow reaction, which shows why high water contents is typically used in the production of foams with lower density [16].

The introduction of amine in the production of flexible polyurethane foam is necessary as it is used up in the startup and maintenance of the reaction between TDI and water, in some cases it is used to compensate for high or low chemical temperatures within certain limits [5].

Table I: Physical and chemical properties of Toluene diisocyanate. (Source: NTP, 2014)

Property	Toluene diisocyanate
Molecular weight	174.2
Specific gravity at 25°C (g/mL)	1.22 or 0.01
Melting point	251°C
LogKow	3.74
Water solubility at 25°C	0.0376g/L
Vapour pressure	2.30 x 10 -2 mm Hg at 25°C
Vapour density relative to air	6

Amine is regarded as blowing catalyst, it accelerates the reaction between isocyanate and water [4].

Stannous Octoate is also one of the chemicals used in the production of flexible polyurethane foam. It is one of the catalysts (organo-tin) used to keep the balance in the reaction process (mostly in the polymerization reaction).

Silicon oil is an essential surfactant needed to control the foaming process, it has two major functions in the production process; to assist in the mixing of the components to form homogeneous liquid and it stabilize bubbles in the rising foam until it cures, this prevent collapse and regulate the open and closed cell character and the pore size of the foam [4, 5].

Methylene chloride is an auxiliary blowing agent used in the production of flexible polyurethane foam to increase the blowing effect during foaming and in the production of soft/lighter foam at all densities [4, 5]. Table 2 shows the summary of influenced physical properties of each chemical during flexible polyurethane foam production.

Table 2: Chemicals and Their Influenced Physical Property (Source: Makanjuola, 1999)

Chemicals	Physical Property Influenced
Polyol	All physical properties
Toluene diisocyanate (TDI)	Hardness
Silicone oil	Cell size, Resilience
Stannous Octoate	Cohesion and hardness
Amine	Catalyst
Water	Density and hardness
Auxiliary blowing agent (methylene chloride)	Density resilience and softness

In order to avoid foam deformity the proportion at which these chemicals mix is of great importance [1]. Table 3 shows possible deformity cause by wrong chemical proportion

Table 3: Foam Deformities And Causes (Source: Arantza, 2005)

Deformities	Meaning and Causes
Sink back	Partial collapse that occurs after attainment of full rise. It is caused by low level of silicon in the formulation or partial/total loss of activity of silicon
Closed foam	This occurs when the inter -connecting spaces between cells are tot ally blocked. It is caused by excess stannous octoate in the formulation, excess silicon, and excess tin catalyst.
Splits	This occurs when cell walls burst which result in series of struts breaking to form a split. It is caused by too little tin catalyst , silicon, too much Amine catalyst and too low TDI index.
Splits and closed foam	It is caused by incorrect balance of the stannous octoate and silicon oil surfactants level. The stannous octoate may be too high, the silicon is too low or both are too low.

2.2 Chemical Proportion Formulation (Cpf) Model Architecture

Chemical proportion formulation determinant (CPF) model has been developed to enhance quality control in flexible polyurethane foam production. The flow chart for the CPF model is as shown in Fig 2. To obtain the required chemical proportion needed for a specified foam density the part by weight (p.b.w) of each chemical must be known. The p.b.w of each of the chemical is based on 100 p.b.w of polyol. For this work four different chemical formulation were done with desired foam mass of 500 kg for foam density 18, 22, 35 and 40 kg/m3. The standard p.b.w of water to foam density used in foam industries is given in Table 4.

Table 4: Standard Specific Proportion Of Foam Density To Water (Source:Mogaji, 2004)

S/N	Water X3 (p.b.w)	Foam Density (Fd) Kg/m3
1	2.0	40
2	2.5	35
3	3.0	30
4	3.5	27
5	4.0	24
6	4.5	20
7	5.0	22
8	5.2	18

2.3 Determination of Chemical proportion

The amount of TDI to react with water and to cure the polyether must be known in order to determine the p.b.w of TDI. The equation for the reaction between TDI and water is given in (1). The p.b.w for polyol, TDI, water, Silicon Oil, Amine and Stannous Octoate are represented with X1, X2, X3, X4, X5 and X6 respectively.

$$y = aX_2 \quad (3)$$

y is the amount of TDI to react with water, α is a constant which is equal to 9.67 (industrial standard) and X3 is p.b.w of water. The amount of TDI to cure the polyether is given by (4)

$$c = hb \quad (4)$$

where;

c is the amount of TDI to cure the polyether , b is a constant which is equal to 0.152 (industrial standard) and h is hydroxyl number of polyol .

The hydroxyl number of polyol depends on the manufacturer and

its ranges within 46 and 47 [5].

p.b.w, X_2 of TDI was calculated using (5)

$$X_2 = \frac{i}{100}(aX_2 + bh) \quad (5)$$

where;

X_2 is p.b.w of TDI and i is TDI index

For flexible polyurethane foam production without Auxiliary Blowing Agent (ABA) TDI index ranges between 106 and 109 to achieve normal hardness [5]

The constraint on p.b.w of silicone oil (X_4) ranges within 0.7 to 1.2 [5]

The p.b.w of Amine (X_5) required can vary generally from 0.12 to 0.30 p.b.w, also, the amount to be used depend on the intensity of the reaction wanted [5]

For density above 25 kg/m3 the p.b.w of Stannous Octoate (X_6) ranges from 0.23 to 0.27 and for density below 25 kg/m3 it ranges from 0.27 to 0.33.

2.4 *Determination of Actual chemical Consumption in kg*

In determining the mass of each chemical to be consumed in a production, the mass of the foam to be produce (k) is of important. In the production of flexible polyurethane foam there are gas losses in the reaction, this makes the mass of the foam produced to be less than the total mass of the chemicals consumed. The gas loss (l) in p.b.w can be calculated using (6)

$$l = rX_3$$

where, l is gas loss in p.b.w and r is a constant.

Equation (7) gives the sum (S) of all p.b.w of chemicals

$$S = \sum_{n=1}^{6} X_n \quad (7)$$

where;

Xn is p.b.w of chemical.

Since chemical proportion of all the chemicals are based on 100 p.b.w of polyol, therefore, assuming 100 kg of polyol in a formulation, actual mass of foam (Ac) in kg to be produced can be calculated using (8)

$$Ac = S - l \quad (8)$$

The multiplying factor (m) for each chemical is given in (9)

$$m = \frac{k}{A_c} \quad (9)$$

The model equation to generate the quantity of each of the chemical in kg is given in (10)

$$`Wn = mX_{n \quad n=1,2,3,4,5,6} \quad (10)$$

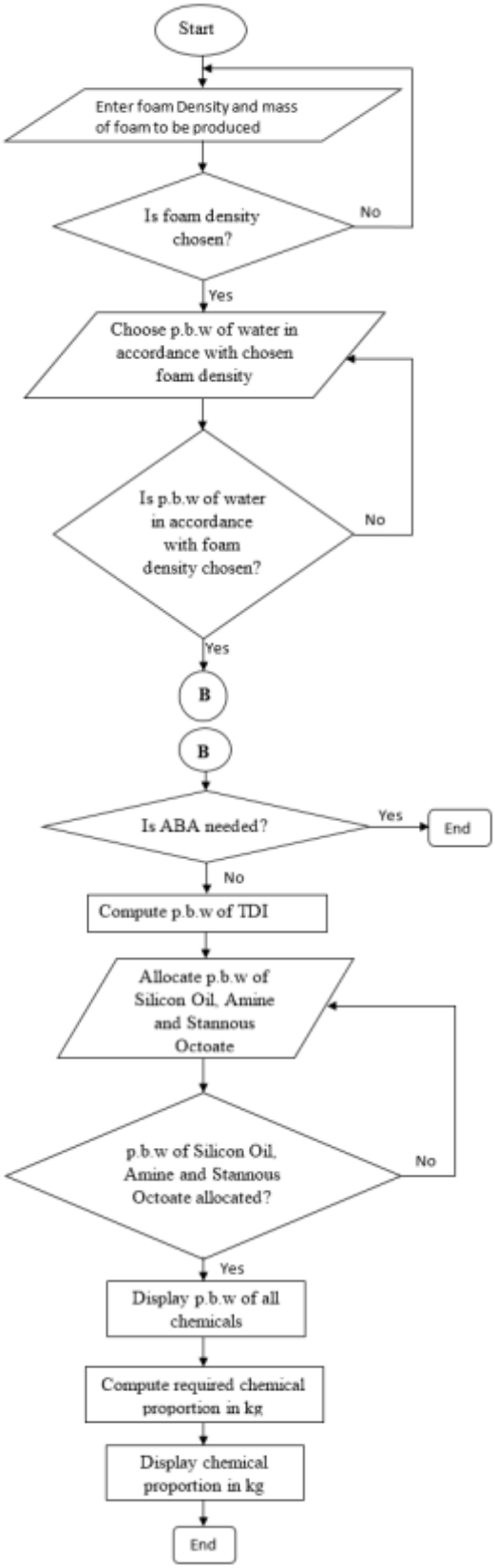


Fig 2 Flow chart for the cpf model developed

where;
Wn is the mass of nth chemical.
Since the number of chemicals considered are six, then,
W1 is the mass of Polyol consumed in kg;
W2 is the mass of TDI consumed in kg;
W3 is the mass of Water consumed in kg;
W4 is the mass of Silicone consumed in kg;
W5 is the mass of Amine consumed in kg and;
W6 is the mass of Stannous Octoate consumed in kg
Now the total mass of the chemical is M kg, then the conduction heat transfer in the mixer chamber is given in (11)

$$q = K\Delta\theta \tag{11}$$

where q is the heat flow rate, Kcal/sec, Δθ is temperature difference, °C and K is the coefficient, Kcal/sec°C. The coefficient K is given (12)

$$K = \frac{\gamma A}{\Delta\zeta} \tag{12}$$

where γ is thermal conductivity of the mixer chamber, Kcal/msec°C, A is the Area normal to heat flow, m2 of the chamber, Δζ is the thickness of the conductor chamber.
The thermal Resistance R for heat transfer between the chemical mixtures is given in (13) and (14)

$$R - \frac{change\ in\ temperature\ difference,\ ^{\circ}C}{change\ in\ heat\ \ flow\ rate,\ Kcal/sec} \tag{13}$$

$$R = \frac{d(\Delta\theta)}{dq} = \frac{1}{K} \tag{14}$$

and the thermal capacitance C of the chamber is defined by (15) and (16)

$$C = \frac{change\ \ in\ heat\ stored,\ KCal}{change\ in\ temperature,\ ^{\circ}C} \tag{15}$$

$$C = M\partial \tag{16}$$

Where M is the mass of the chemical mixtures, kg ∂ is the specific heat of the mixtures, KCal/kg°C.
Since the heat input rate H and the chemical flow rate G are kept constant, then the heat outflow rate will be changed from $\bar{H}$ to $\bar{H}+h_o$ and the temperature of the outflowing chemical will be changed from $\bar{\Theta}_o$ to $\bar{\Theta}_o+\theta$ Then, the heat balance in the mixer chamber is given by (17)

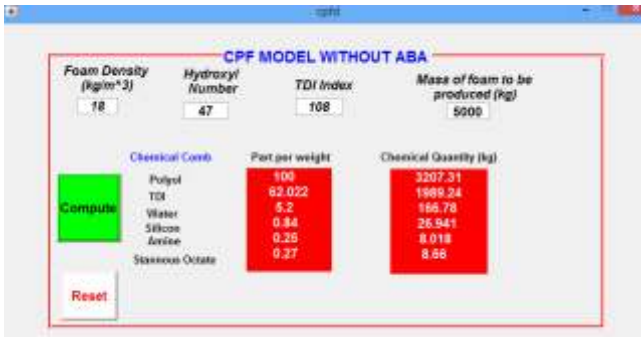
$$c\frac{d\theta}{dt} = (GC\theta_i - h_o) \tag{17}$$

where $\bar{\Theta}_i$ is steady state temperature of inflowing liquid, °C, $\bar{\Theta}_o$ is steady state temperature of outflowing liquid, °C. G is the steady state liquid flow rate, kg/sec, M is the mass of the chemical in mixer chamber, kg. $\bar{H}$ is the steady state heat input rate, Kcal/sec, ho is small change in the heat output rate of the chemical [17].

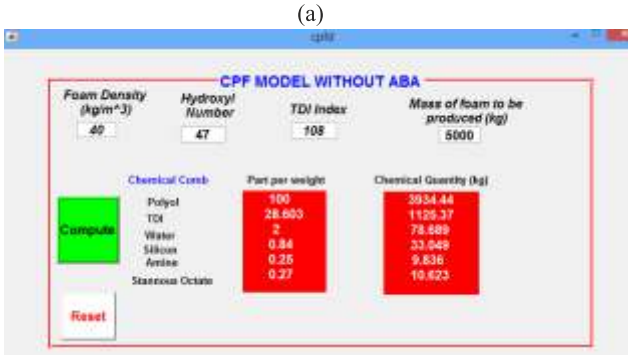
4.0 Result And Discussion

The developed model used (3) to (10) to generate the chemical proportion formulation needed for a specified foam density and foam mass. It provides a GUI for the user to input the foam parameters for the foam to be produced. Sample of the GUI for density 18 and 40 kg/m^3 is shown in Fig. 3
The GUI supply the chemical formulation based on the foam parameter supplied as in Fig. 3, it provides the p.b.w and the chemical quantity needed for the desired foam to be produce. The results generated by the developed model were compared with real life data obtained from a foam industry. The result obtained for foam density 18 kg/m^3 is shown in Fig. 4

The variation between the simulated result and the real life data were seen to be minute in Figure 4 and the difference fall below 10 percent, therefore, it can be said that the model developed is reliable for chemical formulation for a foam density of 18 kg/m3. Similar result was observed for density 22, 35 and 40 kg/m3 as shown in Fig 5 to 7



(a)



(b)

Fig 3: Developed GUI in Matlab/Simulink (a) density 18 kg/m^3 and (b) 40 kg/m^3

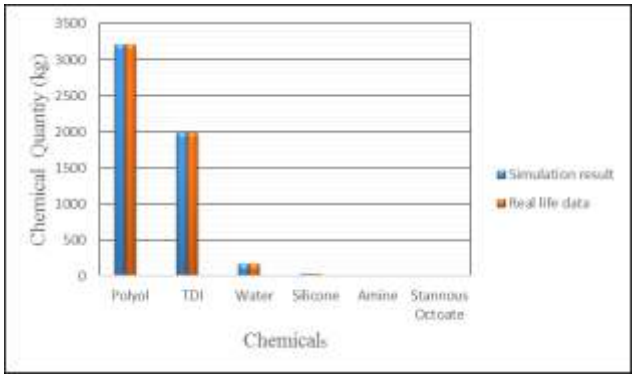


Fig. 4 Comparison for foam density 18 kg/m3

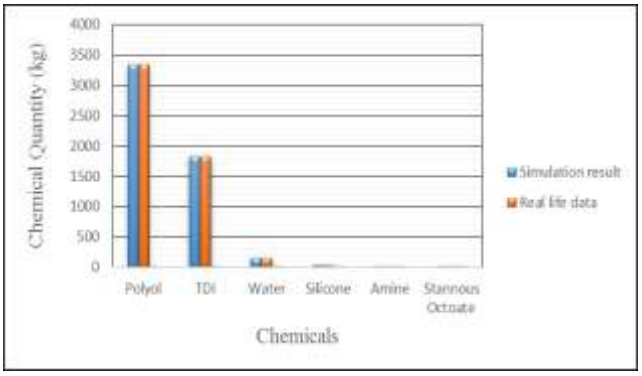


Fig. 5 Comparison for foam density 22 kg/m3

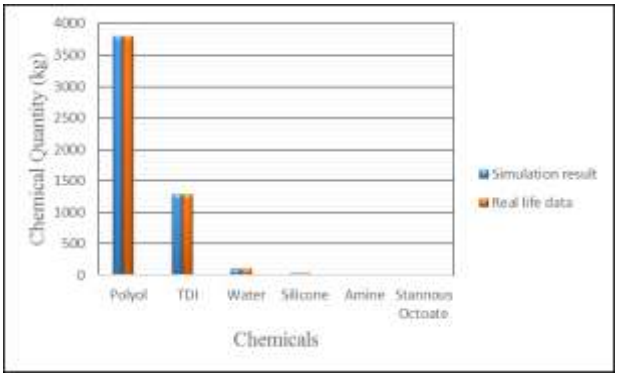


Fig. 6: Comparison for foam density 35 kg/m3

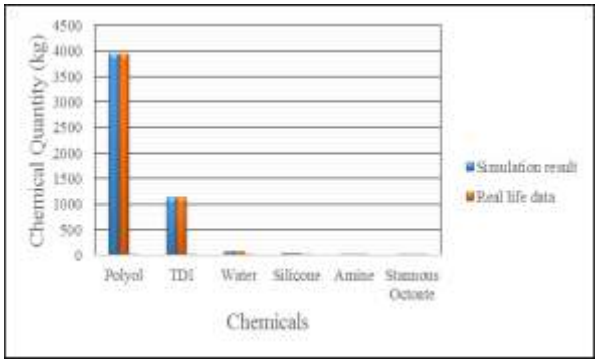


Fig. 7 Comparison for foam density 40 kg/m^3

Table 5: Percentage Difference Between Cpf Mode Result And Real Life Data

	% Difference for Density 18 kg/m3	% Difference for Density 22 kg/m3	% Difference for Density 35 kg/m3	% Difference for Density 40 kg/m3
Polyol	0.032	0.034	0.000	0.016
TDI	0.032	0.033	0.053	0.016
Water	0.032	0.033	0.061	0.011
Silicon Oil	2.401	1.921	1.506	2.308
Amine	0.090	6.716	7.983	0.011
Stannous Octoate	4.128	3.956	3.731	0.028

a. Validation of CPF Model Developed

The performance of the CPF model developed was validated using a two sample t-test for polyol, TDI and water. The percentage difference between the model result and the real life data was determined. The percentage difference shows that there is little or no significant difference between the model result and the real life data. Table 4 shows the percentage difference obtained between the model result and the real life data.

Table 6 is the t-test result for the comparison between the CPF model chemical formulation and real life chemical formulation for polyol, TDI and water. The result shows a 2-tailed significance of 0.215, 0.088 and 0.124 for polyol, TDI and water respectively, which is greater than 0.05 level of significance. This implies that there is no significant difference between the CPF model chemical formulation and real life chemical formulation. Therefore, the CPF model developed can be said to be reliable for chemical formulation in flexible polyurethane foam production. The CPF model developed is faster compare with manual chemical formulation and as well saves time.

Conclusion

A CPF model has been utilized to model chemical formulation in flexible polyurethane foam production. The model developed provides a simple and easy way of generating chemical

Table 6: Two sample t-test result

Polyol				
	t-statistic	t-critical	Df	Sig (2-tailed)
CPF model / Real life data	1.791	4.302	2	0.215
TDI				
	t-statistic	t-critical	Df	Sig (2-tailed)
CPF model / Real life data	3.135	4.302	2	0.088
Water				
	t-statistic	t-critical	Df	Sig (2-tailed)
CPF model / Real life data	2.565	4.302	2	0.124

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